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Improving drought simulations within the Murray-Darling Basin by combined calibration/assimilation of GRACE data into the WaterGAP Global Hydrology Model

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Abstract

1 Simulating hydrological processes within the (semi-)arid region of the Murray-
2 Darling Basin (MDB), Australia, is very challenging specially during droughts.
3 In this study, we investigate whether integrating remotely sensed terrestrial
4 water storage changes (TWSC) from the Gravity Recovery And Climate Exper-
5 iment (GRACE) mission into a global water resources and use model enables a
6 more realistic representation of the basin hydrology during droughts. For our
7 study, the WaterGAP Global Hydrology Model (WGHM), which simulates the
8 impact of human water abstractions on surface water and groundwater stor-
9 age, has been chosen for simulating compartmental water storages and river
10 discharge during the so-called 'Millennium Drought' (2001-2009). In particular,
11 we test the ability of a parameter calibration and data assimilation (C/DA) ap-
12 proach to introduce long-term trends into WGHM, which are poorly represented
13 due to errors in forcing, model structure and calibration. For the first time, the
14 impact of the parameter equifinality problem on the C/DA results is evaluated.
15 We also investigate the influence of selecting a specific GRACE data product

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16 and filtering method on the final C/DA results. Integrating GRACE data into
 17 WGHM does not only improve simulation of seasonality and trend of TWSC,
 18 but also it improves the simulation of individual water storage components. For
 19 example, after the C/DA, correlations between simulated groundwater storage
 20 changes and independent in-situ well data increase (up to 0.82) in three out of
 21 four sub-basins. Declining groundwater storage trends - found mainly in the
 22 south, i.e. Murray Basin, at in-situ wells - have been introduced while sim-
 23 ulated soil water and surface water storage do not show trends, which is in
 24 agreement with existing literature. Although GRACE C/DA in MDB does not
 25 improve river discharge simulations, the correlation between river storage simu-
 26 lations and gauge-based river levels increases significantly from 0.15 to 0.52. By
 27 adapting the C/DA settings to the basin-specific characteristics and reducing
 28 the number of calibration parameters, their convergence is improved and their
 29 and uncertainty is reduced. The time-variable parameter values resulting from
 30 C/DA allow WGHM to better react to the very wet Australian summer 2009/10.
 31 Using solutions from different GRACE data providers produces slightly differ-
 32 ent C/DA results. We conclude that a rigorous evaluation of GRACE errors is
 33 required to realistically account for the spread of the differences in the results.

Keywords: GRACE, WGHM, Data Assimilation, Calibration, Murray
 Darling Basin, Drought

34 **1. Introduction**

35 The Murray-Darling Basin (MDB) in south-eastern Australia is one of the
 36 driest river basins over the world. Long-term hydro-meteorological records indi-
 37 cate that the MDB is prone to extreme hydrological events ([Verdon-Kidd et al.,](#)
 38 [2009](#); [Gallant et al., 2011](#); [Gergis et al., 2012](#)). Particularly, a long drought
 39 period, the so-called ‘Millennium Drought’ ([Ummenhofer et al., 2009](#); [Leblanc](#)
 40 [et al., 2012](#); [van Dijk et al., 2013](#)), occurred during 2001-2009 and affected envi-
 41 ronment, agriculture, and therefore economic activities within the basin. Sub-
 42 sequently, during 2010-2012, the MDB received above average precipitation,

mainly driven by the El Niño Southern Oscillation (ENSO, see e.g., [Boening et al., 2012](#)) and to a smaller extent the Indian Ocean Dipole (IOD, see e.g., [Forootan et al., 2016](#)). Although this helped refilling its terrestrial water storage, studies indicate an overall water availability decline that is likely due to climate change (e.g., [Grafton et al., 2014](#)) noting that the sensitivity of stream-flow generation to changes in climate drivers varies spatially ([Donohue et al., 2011](#)).

Various remote sensing data and hydrological models have been applied to monitor water variability of the MDB. For example, terrestrial water storage changes (TWSC) can be derived from the Gravity Recovery And Climate Experiment (GRACE) satellite mission ([Tapley et al., 2004](#)). The measurements represent the vertical integration of above- and below-surface water storage compartments, and have been used to study the distribution of water and the impact of climate variability within the MDB (e.g., [Brown and Tregoning, 2010](#); [Awange et al., 2011](#); [García-García et al., 2011](#); [Forootan et al., 2012](#)). In addition, remotely sensed surface soil moisture and vegetation water content variations have been analyzed to quantify the influence of large-scale climate variability, such as ENSO and IOD, on the basin hydrology ([Liu et al., 2009](#); [Bauer-Marschallinger et al., 2013](#)). Hydrological models have also been applied over the MDB, such as the WaterGAP Global Hydrology Model (WGHM, [Döll et al., 2003](#)), the Global Land Data Assimilation System (GLDAS, [Rodell et al., 2009](#)), and the high resolution continental model of AWRA (Australian Water Resources Assessment, [van Dijk and Renzullo, 2011](#); [van Dijk et al., 2011](#); [Vaze et al., 2013](#)).

WGHM simulates daily water storage changes in several individual compartments, including canopy, snow, soil, lake, wetland, man-made reservoirs, river and groundwater. The groundwater compartment is often not explicitly realized in other hydrological models (such as GLDAS). In addition, WGHM considers anthropogenic water abstraction, which makes the model distinct from most others. Accurate estimation of water storage variability, including variability of the surface and sub-surface (soil moisture and groundwater) storage compartments, as well as river discharge within the MDB is difficult due to its complex geomorphology, the definition of water connection within the basin ([Lamontagne et al.,](#)

2014), and the strong dependence of hydrology on antecedent rainfall (Beau-
mont, 2012). In general, the simulation skill of hydrological models is limited
by uncertainties in: climate forcing (particularly precipitation), model parame-
ters, and deficiencies in the model structure (Müller Schmied et al., 2014, 2016).
Abelen and Seitz (2013) reported inconsistencies between WGHM and remotely
sensed soil moisture variations, which might be due to neglected physical pro-
cesses. For example, the soil water compartment is defined by a single layer in
WGHM with its depths depending on the plants’ root zone. GLDAS simula-
tions also do not perfectly represent the hydrological property of the MDB due
to the missing groundwater compartment, as well as ignoring the influence of
human water use (e.g., Tregoning et al., 2012). Similarly, the AWRA model does
not account for extensive pumping, which occurs during drought periods. Dur-
ing flood events also, less accurate discharge/recharge estimations are reported
(e.g., in Crosbie et al., 2011). van Dijk and Renzullo (2011) and Forootan et al.
(2012) showed inconsistencies in the linear trend (2003-2011) between GRACE
TWSC and that of AWRA.

To understand the hydrological behavior of the MDB, in most of previ-
ous studies, GRACE TWSC estimates were compared directly to the storage
variability or surface loading estimations simulated by hydrological models or
observed by other techniques e.g., GPS, satellite altimetry, soil moisture remote
sensing, and in-situ observation wells (e.g., Leblanc et al., 2009; Chen et al.,
2016). Variability of a particular storage compartment, e.g., groundwater, is
usually computed by reducing other storage compartments (e.g., surface, canopy
and soil storage compartments) derived from complimentary sources (see an ex-
tensive review in Tregoning et al., 2012, chapter 2). Leblanc et al. (2009), for
instance, conducted a multi-sensor analysis over the MDB, and found a rapid
decline in soil moisture and surface water of about 80 km^3 and 12 km^3 , respec-
tively, during 2001-2003 and low storage levels in the following years. They also
reported that the in-situ groundwater measurements are highly correlated with
GRACE TWSC (correlation coefficients of 0.94) and found a groundwater loss
of about 104 km^3 during 2003-2007. Chen et al. (2016) focused on Victoria,

105 southern Australia, and estimated changes in groundwater by subtracting sim-
106 ulations of the other storage compartments from GRACE TWSC. The authors
107 found a good agreement between their estimations and in-situ observation wells,
108 i.e. a declining trend of about 8.0-8.3 km³/year during 2005-2009.

109 The validity of hydrological assessments in previous works might be limited
110 due to the inconsistencies between GRACE TWSC and model simulations or
111 other observation techniques. Therefore, inversion (e.g., [Forootan et al., 2014](#),
112 [2017](#); [Al-Zyoud et al., 2015](#)) and data assimilation techniques (e.g., [Zaitchik](#)
113 [et al., 2008](#); [Eicker et al., 2014](#); [Van Dijk et al., 2014](#)) should be applied to
114 consistently merge observations with hydrological model simulations.

115 In this study, we pursue the recently improved calibration and data assim-
116 ilation (C/DA) framework based on ensemble Kalman filtering (EnKF, [Schu-](#)
117 [macher et al., 2016](#)) to merge GRACE TWSC estimation with WGHM simu-
118 lations for the MDB. Unlike other hydrological measurements GRACE TWSC
119 constrains the sum of changes within all individual water storage compartments
120 including groundwater, which cannot be measured by any other remote sensing
121 techniques. Using GRACE data, it is not possible to distinguish changes in
122 individual storage components, i.e. whether these changes occur in canopy, soil
123 water, surface water or groundwater. To vertically disaggregate the GRACE-
124 derived TWSC into its individual components, one needs a priori information
125 from other sources, for example, hydrological models, i.e. WGHM in our study.
126 In addition, GRACE observations only provide a coarse horizontal resolution.
127 Data assimilation provides a realistic way to downscale GRACE observations
128 based on the equations implemented in hydrological models. Recently, [Khaki](#)
129 [et al. \(2017a,b\)](#) applied GRACE data and [Tian et al. \(2017\)](#) used GRACE and
130 soil moisture data simultaneously in an ensemble-based assimilation framework
131 to update storage estimation of a hydrological model in Australia and the MDB.
132 Although their studies indicate improvements in soil and groundwater storage
133 estimations, no attempts have been made to calibrate model parameters. In this
134 study, we show to what extent adding water storage information from GRACE,
135 through a C/DA procedure, is able to improve WGHM's TWSC, individual wa-

136 ter storage simulations and its parameters. Hereby, the main focus of our paper
137 is on the effect of the Millennium Drought on the groundwater storage. It is also
138 investigated whether a C/DA of GRACE data affects WGHM's river discharge
139 simulations. This study is the first attempt to assess the impact of GRACE data
140 assimilation on hydrological simulations during a long-term drought period, i.e.
141 here the Millennium Drought.

142 WGHM has 22 parameters that ensure its realistic simulations. However,
143 several parameter combinations may be able to restore observed TWSC and thus
144 GRACE-based calibration alone would be plagued by the equifinality problem.
145 We will show here that, by reducing the number of calibrated parameters, de-
146 ficiencies in model outputs reduces, and subsequently hydrological estimations
147 within the MDB are improved. The implemented C/DA framework has already
148 been successfully applied to improve simulations of total and individual water
149 storage compartments in the Mississippi River Basin (Eicker et al., 2014). Their
150 study was however limited to one year, and the results were not validated with
151 independent data sets. The novelty of the presented framework compared to
152 previous approaches is the extension to model parameter calibration, as well as
153 the implementation of spatial GRACE TWSC error correlations in the ensemble
154 filter update.

155 The objectives of this paper are: (1) to transfer and assess the C/DA ap-
156 proach (Schumacher et al., 2016) to a (semi-)arid region experiencing a severe
157 long-term drought without tuning the approach; (2) to investigate the impact
158 of GRACE data products and its post-processing on the C/DA results; (3) to
159 address the equifinality problem that occurs in the parameter calibration stage;
160 (4) to identify changes in hydrological behavior of the basin within and after
161 the Millennium Drought; and (5) validating the C/DA results using indepen-
162 dent in-situ data, i.e. here river level and river discharge from gauge stations, as
163 well as groundwater well data. The designed objectives will address important
164 technical issues related to the combination of GRACE and hydrological models:

165 Objective (1) will show whether by applying the C/DA and using GRACE

data it is possible to restore long-term trends (water decline in our case) in a particular water storage compartment. This is important since models usually do not realistically represent long-term decline or rising of water levels in the MDB that have been found in GRACE data (Döll et al., 2014). To our knowledge, this is the first application of GRACE-based model parameter calibration via ensemble-based data assimilation for this purpose. An independent validation against in-situ groundwater measurements is also performed.

Objective (2) helps assessing the robustness of the C/DA approach with respect to the choice of data products. This investigation is also important for other studies since there is currently no clear guidance on the “best” selection of a GRACE product and of its post-processing for assimilation studies.

Objective (3) has not yet been tackled in the context of parameter calibration against GRACE data. Therefore, we will discuss how selecting a sub-set of model parameters improves the C/DA.

Objective (4) provides insights about spatial and temporal variations of soil water and groundwater storage changes within the MDB after implementing a C/DA. The combined results are likely more reliable than interpreting WGHM simulations or GRACE data individually.

Objective (5) shows to what extent C/DA can improve water storage simulations and its impact on river discharge simulations can be identified.

2. Study Area and Data

The MDB, with an area of $\sim 1,060,000 \text{ km}^2$, is home of two major rivers; the Murray River and the Darling River, which joins the Murray River around 500 km upstream from the basin outlet. It extends from the subtropics of central Queensland to the southern alps of Victoria and the Southern Ocean, therefore, it has been under influence of both humid and arid climates and their variabilities (Connell and Grafton, 2011). Most of the basin is flat, low-lying

and far inland, and receives 477 mm area-averaged annual rainfall (Fu et al., 2010). Its tributary rivers tend to be long and slow-flowing, and carry a volume of water that is large only by Australian standards. The sedimentary rocks have a maximum depth of 600 m; thus, groundwater storage is relatively small. The MDB is essentially a closed groundwater basin, where groundwater drainage is directed internally towards the central subsidence and thicker sediments, rather than towards the side where the Murray connects to the sea (Grafton et al., 2014).

We consider four sub-basins within the MDB: the arid north-western Darling area (NW), which contains the Darling and Warrego Rivers, and the north-eastern Darling area (NE) in which the Balonne River and several other northern rivers flow. The other two consist of the south-eastern Murray area (SE) with the first half of the Murray River, and the whole Lachlan and Murrumbidgee Rivers, as well as the south-western Murray area (SW) with the second half of the Murray River. These regions are defined (i) based on the hydrological sub-basins and underlying river routing system considered in WGHM, as well as (ii) the spatial area detectable by GRACE. The shapes of the sub-basins and their areas are reported in Fig. 1.

2.1. Hydrological Model: WGHM

The WaterGAP Global Hydrology Model (WGHM) and five water use models together form the global water availability and use model Water - Global Assessment and Prognosis (WaterGAP). WGHM uses a number of water storage equations that describe the daily vertical water balance and horizontal routing, with a spatial resolution of $0.5^\circ \times 0.5^\circ$ for the global land area excluding Antarctica. Detailed descriptions of the model equations are given in Döll et al. (2003) and Müller Schmied et al. (2014). In this study, we use the model version WaterGAP 2.2 for calibration and data assimilation (C/DA) of GRACE TWSC. The model has already been calibrated against mean annual river discharge at 1319 Global Runoff Data Centre (GRDC) stations, of which 11 are located in the MDB (Müller Schmied et al., 2014). The monthly forcing fields of tempera-

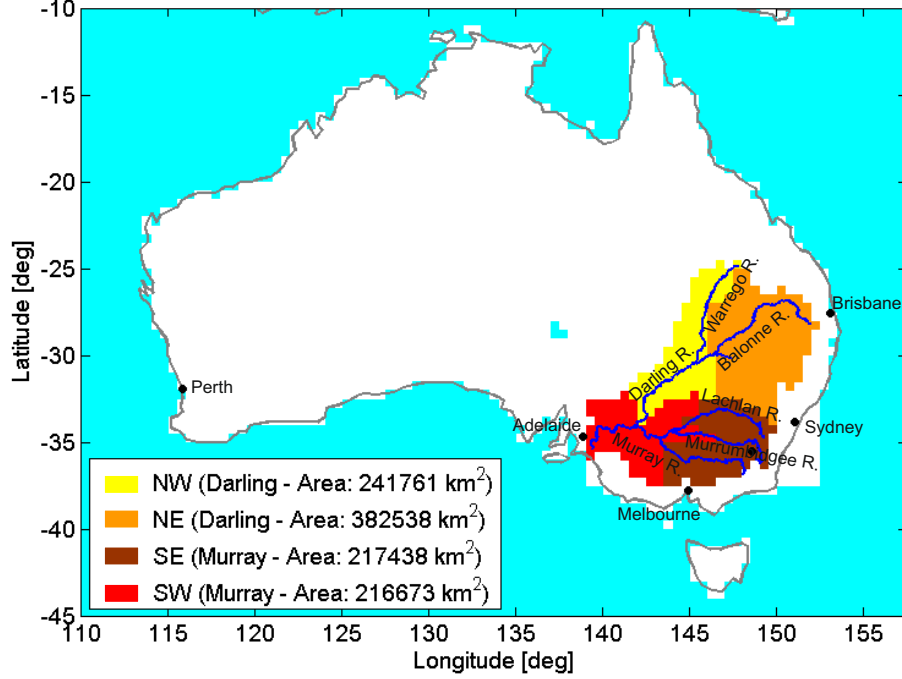


Figure 1: The Murray-Darling Basin (MDB) and its four sub-basins considered here to integrate GRACE TWSC with the WGHM model simulations.

ture, cloud cover, and the number of wet days were obtained from the Climate Research Unit's Time Series (CRU TS 3.2; Harris et al., 2013) and precipitation provided by the Global Precipitation Climatology Center (GPCC v6; Schneider et al., 2014), which at the date of our study were available until end of 2010.

2.2. GRACE TWSC

Monthly GRACE level 2 products, expressed as dimensionless spherical harmonics of the geopotential up to degree and order 90, are available from different sources. Here, the RL05 of GFZ and JPL (<ftp://podaac-ftp.jpl.nasa.gov/allData/grace/L2/>) are considered, as well as those of ITSG-Grace2014 (http://portal.tugraz.at/portal/page/portal/TU_Graz/Einrichtungen/Institute/Homepages/i5210/research/ITSG-Grace2014). Degree 1 coefficients are replaced by those from Swenson et al. (2008). The zonal degree 2 spherical har-

monic coefficients (C_{20}) are replaced by Satellite Laser Ranging (SLR) data (Cheng et al., 2013, see also grace.jpl.nasa.gov).

GRACE level 2 products contain correlated errors, visible as striping patterns in the spatial domain (Kusche, 2007). Therefore, before computing monthly TWS fields, the DDK3 anisotropic decorrelation filter (Kusche et al., 2009) is applied to suppress such errors. Monthly residual gravity field solutions are computed by subtracting the temporal average of 2003-2010 from each month. The residual coefficients are then converted to gridded TWSC fields (on the $0.5^\circ \times 0.5^\circ$ grid used in WGHM) following Wahr et al. (1998). The same steps are repeated for the ITSG-Grace2014 product, while applying a Gaussian filter with 300 km and 500 km radii to investigate the influence of smoothing of GRACE TWSC on the C/DA results. A formal variance-covariance error propagation is carried out to obtain the observation error covariance matrices (Schumacher et al., 2016). It is worth mentioning that the TWSC estimations from CSR data lie within the GRACE ensemble (ITSG-GRACE2014, GFZ, JPL). Thus, here, we do not explicitly report the results based on CSR data. In total, five different GRACE TWSC variants are considered in this study. For all variants, the full error covariance matrix of the ITSG-Grace2014 product smoothed by a 300 km Gaussian filter is used.

For the C/DA, Schumacher et al. (2016) suggest to integrate GRACE TWSC and model simulations either on coarse grids, e.g., $5.0^\circ \times 5.0^\circ$ or as (sub-) basin averages. In this study, we select GRACE TWSC averaged over the four sub-basins of Fig. 1 for assimilation into WGHM. To account for the signal damping and spatial leakage due to the application of filtering, constant and time-variable scaling factors are estimated (see Sect. 6 of the Supplementary Data for details). The scaling values are found to be close to 1. The main C/DA results are presented with respect to the ITSG-Grace2014 product, which is filtered by DDK3, and called ITSG-DDK3 in the following.

265 2.3. Groundwater Observations

266 Groundwater changes from around 15800 observation wells within the MDB
267 are applied to validate the C/DA results. The measurements were spatially
268 averaged over $1^\circ \times 1^\circ$ grid cells, including between one to around 2680 wells
269 per grid cell. The locations of the individual observation wells are provided in
270 (Tregoning et al., 2012). It was reported that these wells might be influenced
271 by local effects such as pumping that might cause draw-down or recharge due to
272 irrigation. The observations are expressed as groundwater levels, and converted
273 to equivalent water heights (EWH) by considering aquifer specific yield, which is
274 usually unknown and cannot be measured at this scale. Here, we use an estimate
275 of 0.1 as a typical value for water aquifers as proposed by Tregoning et al. (2012).
276 To demonstrate the effect of the choice of the specific yield, additionally specific
277 yield maps based on surface geology are considered (Viney et al., 2015, , Sect.
278 4.3.2).

279 3. Calibration and Data Assimilation (C/DA) Framework

280 An overview of the calibration and data assimilation (C/DA) study set-up is
281 given in Fig. 2. To run the hydrological simulation, WGHM is initialized during
282 1995-2000. Then, an ensemble of $N_e=30$ runs is generated to represent uncer-
283 tainties in forcing data, model parameters (see Tab. 1), initial water states and
284 errors in the model structure. For this, a priori Probability Density Functions
285 (PDF) are considered for the model parameters based on literature (Döll et al.,
286 2003; Kaspar, 2004; Schumacher et al., 2015). A multiplicative error model is
287 assumed for precipitation fields centered around 1 and with limits of 0.7 and
288 1.3, and an additive error model for temperature fields centered at 0 and limits
289 of $\pm 2^\circ\text{C}$; both are added as white noise. The generated ensembles are used in
290 a two years model spin-up phase during 2001-2002 to generate an ensemble of
291 initial water states. Our experiments with the initialization and spin-up length
292 indicate that these have negligible influence on the model runs (details in Sect.
293 7, Supplementary Data.

294 First, an open loop (OL) run during 2003-2010, i.e. WGHM runs are per-
 295 formed with each of the 30 ensemble members (first column in Fig. 2, and Tab.
 296 2). Within WGHM, parameter values are set globally, i.e. the same values are
 297 used in all river basins world-wide. Moreover, the parameters are temporally
 298 constant. Subsequently, WGHM is run in C/DA mode, i.e. GRACE TWSC
 299 observations along with their full error covariance information are assimilated
 300 monthly into WGHM (second column in Fig. 2, and Tab. 2) using the EnKF
 301 (Evensen, 1994; Burgers et al., 1998). In the EnKF updates, the water mass
 302 balance is not conserved, i.e. water mass can be introduced to or removed from
 303 WGHM. By applying the C/DA, model parameters are calibrated sequentially
 304 each time that GRACE observations are available within the MDB. Therefore,
 305 the calibrated parameters are the most appropriate for the MDB but not nec-
 306 essarily for other river basins. The adjusted parameter values are then used to
 307 start the WGHM runs for the next months. This is done for the entire 2003-
 308 2010. In summary, parameter values after the C/DA vary in time and are not
 309 identical to the parameters used in the OL run. Since the updated water states
 310 and parameters are adjusted to the GRACE observations within each EnKF
 311 update step, the model uncertainties decrease successively. Thus, an inflation
 312 factor of 10%, based on findings in Schumacher et al. (2016), is used to ensure
 313 a contribution of GRACE TWSC to the updated water states and parameters
 314 during the entire study period (addressing Objective 1).

315 We also carry out five experiments with a range of configurations (Tab. 2):
 316 (i) different GRACE products (ITSG, GFZ, JPL) are used for introducing the
 317 observed TWSC, and (ii) various spatial filters applied to the ITSG-Grace2014
 318 data product (300 and 500 km Gaussian filter, as well as DDK3), to account for
 319 the impact of GRACE post-processing (addressing Objective 2).

320 Another experiment is designed, in which only the three parameters of the
 321 root depth multiplier, net radiation multiplier and groundwater outflow coeffi-
 322 cient are calibrated instead of the 22 model parameters (C/DA (v2) in Tabs. 1
 323 and 2). These three parameters are selected since they are relatively indepen-
 324 dent and have considerable influence on simulating relevant water compartments

325 in the MDB, i.e. soil water and groundwater. By this reduction and compar-
 326 ing to the C/DA version, in which all 22 parameters are calibrated, we can
 327 investigate the equifinality problem using GRACE TWSC for model calibration
 328 (addressing Objective 3).

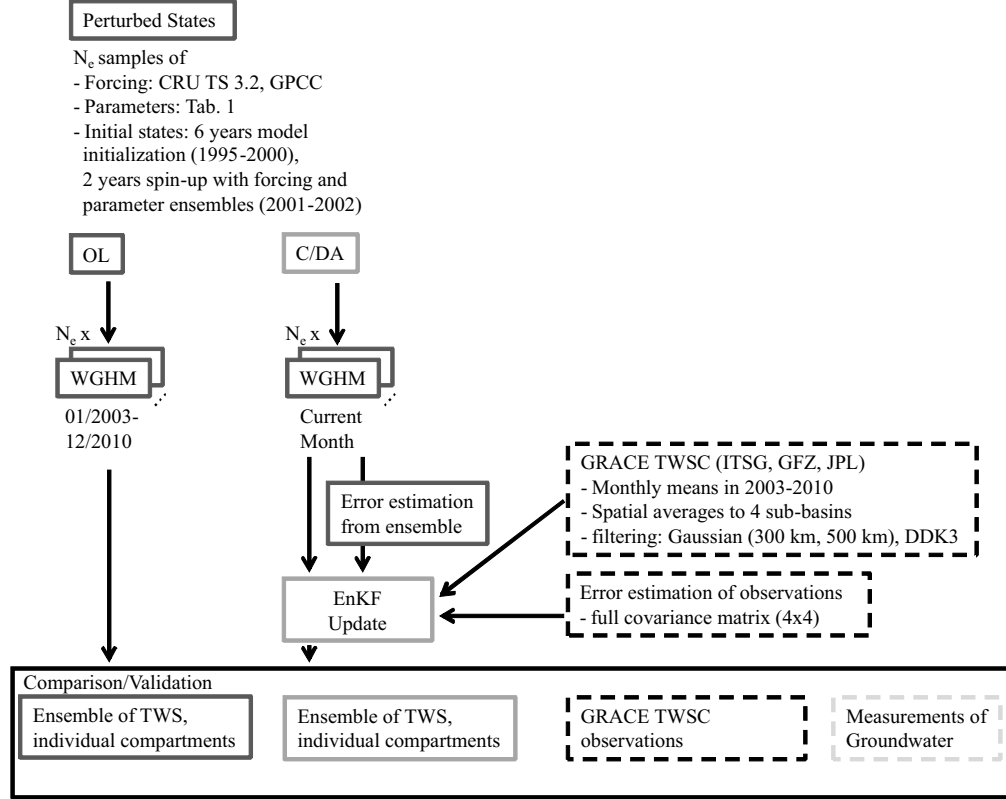


Figure 2: Set-up of study for the Murray-Darling Basin (MDB). First, open loop (OL) model runs are performed over 2003-2010 (left column). Subsequently, GRACE TWSC averaged over the 4 major sub-basins of the MDB are assimilated into WGHM testing different configurations (center and right column) and simultaneously the WGHM's parameters are calibrated (see Tab 1). To assess the C/DA results, simulated TWSC and groundwater changes are compared to GRACE TWSC and independent groundwater well measurements.

Table 1: Model parameters that are calibrated within the EnKF, where “IN” indicates the identification number, “mode” represents the value used in the original WGHM run, and under “limits” the spread of parameter values used for ensemble generation are summarized. The last two columns indicate whether a parameter is calibrated against GRACE. For the C/DA version 2 (v2) run, the mode and limits of parameters 3, 4 and 19 are modified. These values are provided in brackets.

IN	Calibration Parameter	Mode	Limits	C/DA	C/DA (v2)
1	root depth multiplier	1	[0.5 2.0]	yes	yes
2	river roughness coefficient multiplier	1	[0.5 2.0]	yes	-
3	lake depth (m)	5 (4)	[1 20] ([1 10])	yes	-
4	wetland depth (m)	2 (1)	[0.5 5] ([0.5 2])	yes	-
5	surface water outflow coefficient (day ⁻¹)	0.01	[0.001 0.1]	yes	-
6	net radiation multiplier	1	[0.5 2.0]	yes	yes
7	Priestley-Taylor coefficient (humid)	1.26	[0.885 1.65]	yes	-
8	Priestley-Taylor coefficient (arid)	1.74	[1.365 2.115]	yes	-
9	maximum daily potential evapotranspiration (mm/day)	15	[7.25 22.5]	yes	-
10	maximum canopy water height per leaf area (mm)	0.3	[0.1 1.4]	yes	-
11	specific leaf area multiplier	1	[0.5 2.0]	yes	-
12	snow freeze temperature (°C)	0	[-1.0 3.0]	yes	-
13	snow melt temperature (°C)	0	[-3.75 3.75]	yes	-
14	degree day factor multiplier	1	[0.5 2.0]	yes	-
15	temperature gradient (°C/m)	0.006	[0.004 0.01]	yes	-
16	groundwater recharge factor multiplier	1	[0.5 2.0]	yes	-
17	maximum groundwater recharge multiplier	1	[0.5 2.0]	yes	-
18	critical precipitation for groundwater recharge (mm/day)	10	[2.5 20.0]	yes	-
19	groundwater outflow coefficient (day ⁻¹)	0.006 (0.01)	[0.006 0.018] ([0.004 0.016])	yes	yes
20	net abstraction surface water multiplier	1	[0.5 2.0]	yes	-
21	net abstraction groundwater multiplier	14 1	[0.5 2.0]	yes	-
22	precipitation multiplier	1	[0.8 1.2]	yes	-

Table 2: Overview of model simulations and assimilation runs that are analyzed in this study. The main results are presented with respect to the C/DA variant ITSG-DDK3 and the C/DA version 2 (v2), in which only three model parameters are calibrated (see Tab. 1). The remaining C/DA variants are discussed in the Supplementary Data.

Run	Method	GRACE Product	GRACE Filtering
OL	Open Loop	-	-
ITSG-DDK3	EnKF	ITSG-Grace2014	DDK3
ITSG-300km	EnKF	ITSG-Grace2014	300 km Gaussian
ITSG-500km	EnKF	ITSG-Grace2014	500 km Gaussian
GFZ-DDK3	EnKF	GFZ RL05	DDK3
JPL-DDK3	EnKF	JPL RL05	DDK3
C/DA (v2)	EnKF	ITSG-Grace2014	DDK3

4. Results

4.1. Meteorological and Hydrological Conditions

During the Millennium Drought (2001-2009), the MDB has received below average precipitation (see e.g., [Leblanc et al., 2012](#); [van Dijk et al., 2013](#)). Basin-averaged annual precipitation from the Australian Bureau of Meteorology (BoM) during 1981-2013 shows that 2001-2009 was the longest period with below the mean precipitation of 477 mm (Fig. 3 (A), see also [Forootan et al., 2016](#)). Compared to the previous three decades, particularly, 2002 and 2006 were the driest years with up to 41% below average precipitation, followed by the wettest year in 2010 with 66% higher annual precipitation. The distribution of precipitation is however not homogeneous over the basin. In Fig. 3 (B), the differences between the mean annual precipitation over the Millennium Drought, and during 1981-2013 are shown on a $0.5^\circ \times 0.5^\circ$ grid. In the Darling Basin (northern part), precipitation is found to be overall higher during 2001-2009 compared to the three decade mean with a maximum value of +38 mm/year. In contrast, precipitation in the Murray Basin (southern part) is

345 found smaller with a maximum of -40 mm/year. Therefore, we expect strong
 346 impact from the meteorological drought predominantly in the south.

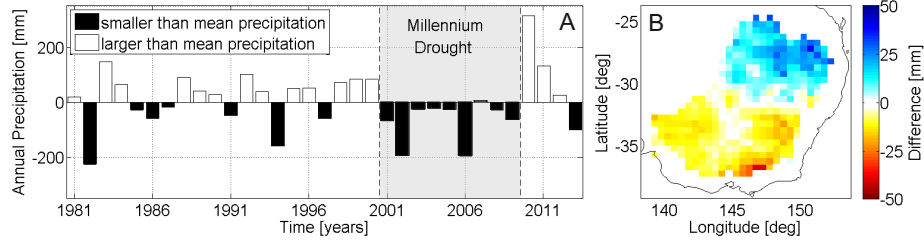


Figure 3: (A) Divergence of annual precipitation in mm (from the long-term temporal mean of 477 mm) averaged over the entire Murray-Darling Basin (MDB). (B) Difference in mean annual precipitation during 2001-2009 and 1981-2013 on a $0.5^\circ \times 0.5^\circ$ grid.

347 In Fig. 4, monthly TWSC derived from the open loop (OL) run during
 348 1995-2010 and from GRACE during 2003-2013 over the entire MDB are shown.
 349 The WGHM simulation shows a strong decline in TWSC during 2001-2002,
 350 as well as a strong increase in 2010, which are clearly related to the extreme
 351 meteorological conditions. However, no further water decline is visible in the
 352 very dry year 2006. In contrast, during 2003-2007, the GRACE-derived TWSC
 353 decreased and is found mostly below the temporal mean until 2009. The strong
 354 rainfall events in 2010 and 2011 resulted in an increase of the total water mass
 355 (Forootan et al., 2012). Afterwards, TWSC values are found to be mostly above
 356 the temporal mean.

357 No significant linear trend is visible in TWSC from the WGHM OL run dur-
 358 ing 2003-2009. On the contrary, the estimation from the ITSG-DDK3 GRACE
 359 solution (see Tab. 2) shows a decrease of -7.6 mm/year over the entire MDB,
 360 ranging from -2.9 mm/year in the north-eastern Darling Basin (NE) to -14.0
 361 mm/year in the south-eastern Murray Basin (SE, Tab. 3). Although precipita-
 362 tion is above the three decadal average (see Fig. 3 (B)), the linear trends in the
 363 Darling Basins are found to be negative. The application of different filtering to
 364 smooth GRACE TWSC represents a small impact on the linear trend estima-
 365 tion in the Darling sub-basins (differences of around 0.3 mm/year, see column

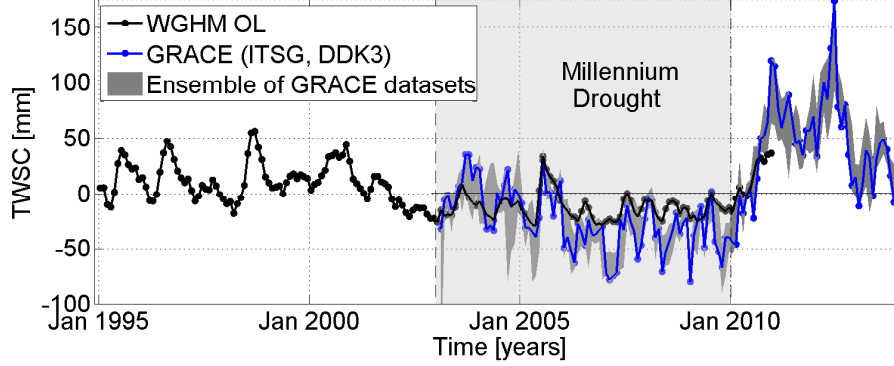


Figure 4: TWSC (in mm) derived from the WGHM open loop (OL) run and from GRACE averaged over the entire Murray-Darling Basin (MDB). The black line shows the WGHM OL, the blue line indicates GRACE (using ITSG-Grace2014), which is smoothed by the DDK3 filter, while the dark gray area represents the range of all investigated GRACE datasets (see Tab. 2).

366 “GRACE Filtering” in Tab. 3), and a higher influence in the Murray sub-basins
 367 (differences of up to 3.0 mm/year, see Tab. 3). Using different GRACE prod-
 368 ucts for the trend estimation has a similar impact on the results (see column
 369 “GRACE Products” in Tab. 3). However, all analyzed GRACE data sets in-
 370 dicate negative trends in TWSC for the entire MDB. Therefore, an improved
 371 representation of the TWSC decline between 2003-2009 is expected by merging
 372 GRACE and WGHM in the C/DA framework.

373 4.2. TWSC Simulations from WGHM

374 4.2.1. Improving the Representation of TWSC

375 TWSC time series from the open loop (OL) simulations, GRACE and the cal-
 376 ibration and data assimilation (C/DA) results after assimilating ITSG-DDK3,
 377 are shown in Fig. 5. A much better agreement is found between C/DA results
 378 (and the ensemble of all C/DA variants) with GRACE TWSC compared to the
 379 OL variant of WGHM. In terms of root mean square errors (RMSE), the fit for
 380 the entire basin is improved by 50% (from 21.4 to 10.7 mm), ranging from 45%
 381 in the north-western Darling Basin (NW) to 53% in both Murray sub-basins

Table 3: Linear trend (in mm/year) during 2003-2009 and its error derived by ITSG-Grace2014 (filtered by DDK3) for the averages over the entire MDB and its four major sub-basins (see the basins in Fig. 1). Averaged linear trends and their uncertainties estimated from different GRACE products, as well as after applying different filtering techniques are presented.

Basin	ITSG-DDK3	GRACE	GRACE
		Products	Filtering
MDB	-7.6 ± 0.6	-5.9 ± 1.5	-6.8 ± 1.0
NW	-3.8 ± 0.8	-2.7 ± 1.0	-4.2 ± 0.3
NE	-2.9 ± 0.8	-0.8 ± 2.1	-3.2 ± 0.3
SE	-14.0 ± 0.7	-11.7 ± 2.1	-11.1 ± 3.0
SW	-13.5 ± 0.7	-12.8 ± 0.6	-11.4 ± 2.4

(Tab. 4). Applying different filtering techniques or using different GRACE products indicate improvements for the entire basin of up to 51% in terms of RMSE with respect to the OL variant. Furthermore, the correlation coefficient of WGHM simulated TWSC after C/DA with GRACE TWSC improves by 37% (from 0.58 to 0.92) for the entire MDB compared to OL. For the sub-basins, the improvements range between 28% in the south-eastern Murray Basin (SE) and 72% in the north-western Darling Basin (NW). Assessing the different C/DA variants in Tab. 2 indicates improvements for the entire MDB in terms of correlation coefficients of up to 36% compared to OL. After calibrating only three model parameters in C/DA (v2), the correlation coefficients are still high and the RMSE has been reduced compared to the OL. The individual RMSE and correlation coefficient values of all C/DA variants can be found in Tabs. S1 and S2 of the Supplementary Data.

The influence of assimilation on WGHM in simulating TWSC on the $0.5^\circ \times 0.5^\circ$ grid is assessed in Fig. 6, which shows correlation coefficients and RMSE between model simulations (from OL and C/DA) and GRACE TWSC after applying DDK3 filtering for both. Low to moderate improvements in correlations are found after C/DA all over the basin. The RMSE values between the WGHM

400 simulated TWSC after C/DA and GRACE TWSC are found also to be smaller
401 compared to the OL variant.

Table 4: Agreement between model predicted and observed TWSC in terms of correlation coefficients (CC) and root mean square errors (RMSE) in mm. Improvements are reported in the brackets.

	CC		CC		RMSE		RMSE	
Basin	OL	ITSG-DDK3	C/DA (v2)		OL	ITSG-DDK3	C/DA (v2)	
MDB	0.61	0.92 (+0.31)	0.87 (+0.26)		21.7	10.7 (-11.0)	13.3 (-8.3)	
NW	0.23	0.75 (+0.52)	0.58 (+0.36)		23.3	15.7 (-7.6)	19.0 (-4.2)	
NE	0.45	0.89 (+0.44)	0.79 (+0.34)		27.8	14.7 (-13.1)	19.4 (-8.4)	
SE	0.73	0.95 (+0.22)	0.93 (+0.20)		30.2	13.7 (-16.5)	16.3 (-14.0)	
SW	0.52	0.91 (+0.39)	0.83 (+0.30)		33.8	16.1 (-17.7)	22.1 (-11.8)	

402 4.2.2. Linear Trends and Seasonality in TWSC

403 The estimated linear trends in TWSC from the OL and C/DA variants
404 of WGHM are summarized in Tab. 5. The standard deviations of the WGHM
405 variant ITSG-DDK3 and C/DA (v2) are determined by formal error propagation
406 based on the error covariance matrices of the EnKF updates. A comparison of
407 the trends after C/DA with the trends from OL, and different GRACE products
408 shows that the negative trends in the WGHM TWSC are reasonably intensified.
409 The mean difference of the trends from the C/DA variants compared to GRACE
410 is 1.5 mm/year, while the mean difference to the TWSC outputs of the OL
411 simulations is 5 mm/year. The trends of the C/DA (v2) variant are somewhat
412 smaller in the western parts of the MDB.

413 In order to assess whether the contribution of GRACE TWSC in the updated
414 WGHM simulations (after C/DA) is realistically distributed, in Fig. 7, we show
415 those statistically significant linear rates in TWSC that are found in the MDB
416 during 2003-2009. A t-test with a significance level of 97.5 % is applied for this

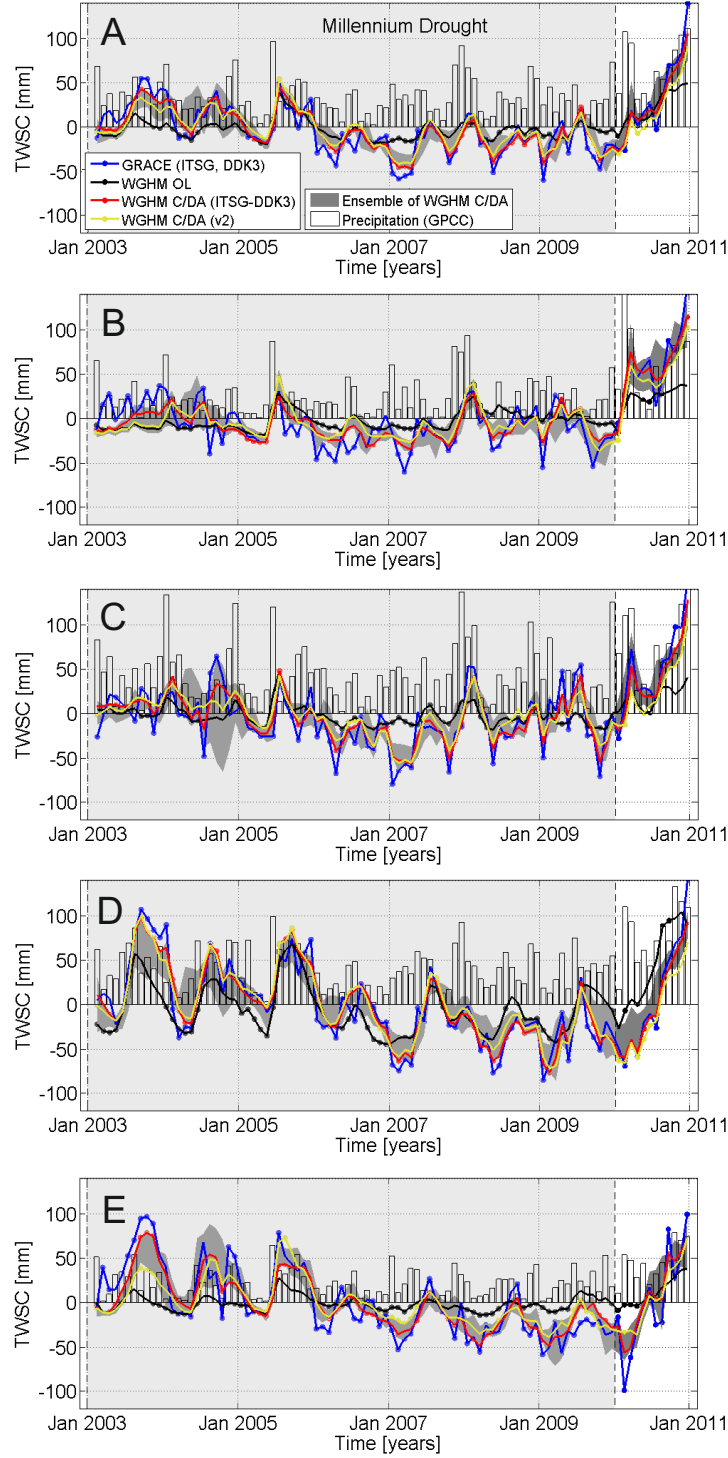


Figure 5: Monthly TWSC in mm averaged (A) over the entire MDB, (B) over NW, (C) over NE, (D) over SE, and (E) over SW. The blue line indicates the TWSC from GRACE (ITSG, DDK3); the black line indicates the WGHM OL simulation; the red line indicates the WGHM simulation after C/DA of GRACE (ITSG, DDK3), and the yellow line the WGHM simulation after C/DA (v2) of GRACE (ITSG, DDK3). The dark gray area represents the range of all C/DA results (see Tab. 2 for C/DA configurations).

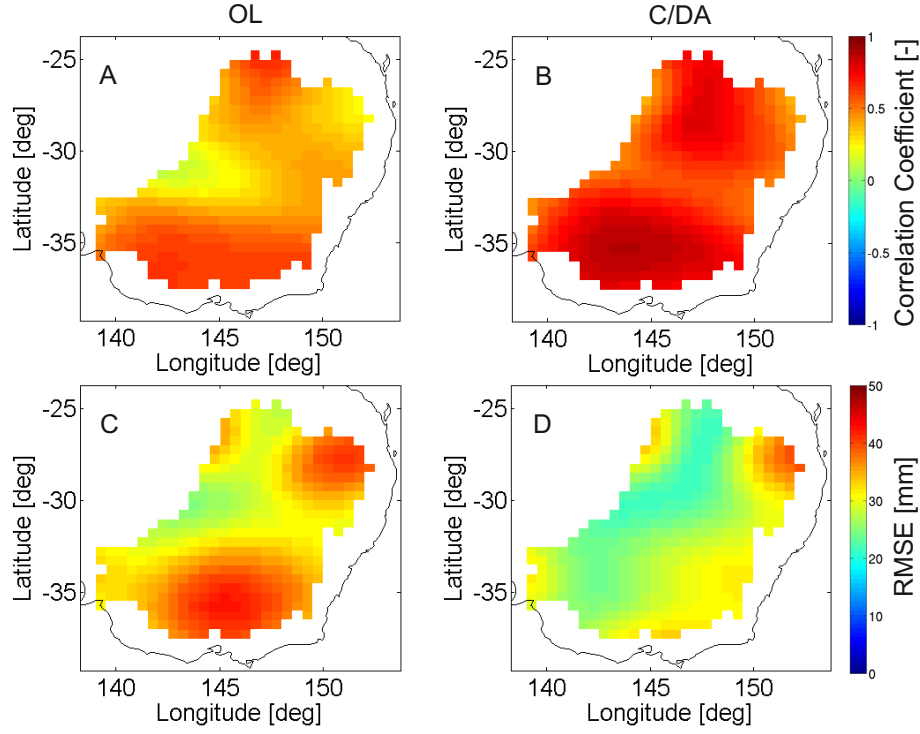


Figure 6: Gridded correlation coefficients between WGHM TWSC simulation and ITSG-Grace2014 TWSC after applying DDK3 filtering for both; (A) for the OL, (B) after applying the C/DA. Gridded root mean square error (RMSE) in mm estimated (C) from the differences between OL TWSC and those of GRACE, and (D) from the C/DA TWSC and GRACE TWSC.

assessment. As it was expected from the basin averaged results (Fig. 4), the DDK3-filtered OL TWSC does not contain significant linear trends (see Fig. 7 (A)), while in the non-smoothed simulations, moderate negative trends can be found over parts of the north and south-west of the MDB (see Fig. 7 (D)). After applying the C/DA based on ITSG-DDK3, a negative trend in TWSC is introduced mainly to the south, which can be seen in Fig. 7 (B) and (E). The restored linear trends (Fig. 7 (B)) are in better agreement with those of GRACE compared to the OL simulation (Fig. 7 (C)).

Our results indicate that the CD/A also influences the seasonal skill of WGHM. In Fig. 8, the annual amplitude of TWSC for 2003-2009 is shown. The DDK3-filtered values, estimated from the OL, C/DA, and ITSG-Grace2014, are shown in Fig. 8 (A), (B), and (C), respectively. Comparing the spatial distri-

429 butions and magnitude of the annual cycle, one can easily see that the C/DA
430 results (in B) are tuned towards GRACE estimation (in (C)) compared to those
431 of the OL (in A). In Fig. 8 (D) and (E), the annual amplitudes of TWSC,
432 without applying a filter, are shown, which indicate that the OL simulation
433 underestimates the annual cycle mainly over the south and north-east (Fig. 8
434 (D)). This is however improved after applying C/DA (see Fig. 8 (E)).

Table 5: Linear trends (in mm/year) of TWSC and their uncertainty during 2003-2009 computed for the entire MDB and the four sub-basins (basins are shown in Fig. 1). The OL results and those after the C/DA of WGHM using ITSG-Grace2014-DDK3 are shown in the second and third columns, respectively. The averages of linear trends and their errors from different GRACE products, and after applying different filtering techniques are reported in the fourth and fifth columns, respectively. Results of the C/DA (v2) is reported in the last column.

Basin	OL	ITSG-DDK3	GRACE Products	GRACE Filtering	C/DA (v2)
MDB	-0.9 ± 0.05	-6.5 ± 0.3	-5.3 ± 1.6	-5.7 ± 1.1	-5.5 ± 0.1
NW	2.1 ± 0.09	-1.0 ± 0.2	-0.8 ± 1.0	-2.0 ± 1.0	-0.3 ± 0.2
NE	-1.6 ± 0.04	-4.2 ± 0.5	-2.3 ± 2.1	-3.9 ± 0.4	-3.8 ± 0.1
SE	-3.7 ± 0.13	-13.0 ± 0.7	-10.9 ± 2.5	-9.7 ± 3.4	-12.2 ± 0.2
SW	-0.4 ± 0.11	-10.0 ± 0.3	-9.7 ± 0.6	-9.0 ± 1.8	-7.3 ± 0.1

435 4.3. Details of Groundwater Storage Changes

436 4.3.1. Improvements of the Representation of Groundwater Changes

437 Among various water storage compartments simulated by WGHM, our re-
438 sults indicate that the negative linear trends, restored in WGHM by assimilating
439 GRACE TWSC, are predominantly associated with the groundwater compart-
440 ment, and much less with the surface water and soil water storage compartments
441 (see the results of the surface and soil compartments in the Supplementary Data,
442 Figs. S1 and S2). While in [van Dijk et al. \(2013\)](#) a decrease in public reservoirs
443 is reported for 2006-2007, our analysis agrees well with the findings in [Leblanc](#)

et al. (2009), who did not find considerable trend in surface water and soil moisture in MDB since 2003. This comparison does not allow to distinguish whether OL or the C/DA results are better. However, it clearly shows that C/DA did not erroneously introduce decreasing trends to the soil and surface water components (as could have happened given the decreasing trend in TWSC). This was, however, correctly translated by C/DA to a water decline in the groundwater storage only.

In Fig. 9, WGHM's groundwater time series (derived by OL runs and after C/DA) and the observed groundwater well time series are shown. Results are averaged over the entire MDB and its four sub-basins of Fig. 1. All graphs in Fig. 9 (A) to (E) indicate nearly constant values in the OL simulations (black lines), which are not consistent with the well measurements (blue lines) that show strong annual variability and linear trends within most sub-basins. After C/DA, the agreement of simulated and observed groundwater is clearly improved for the entire MDB and all four sub-basins: Seasonal variability and

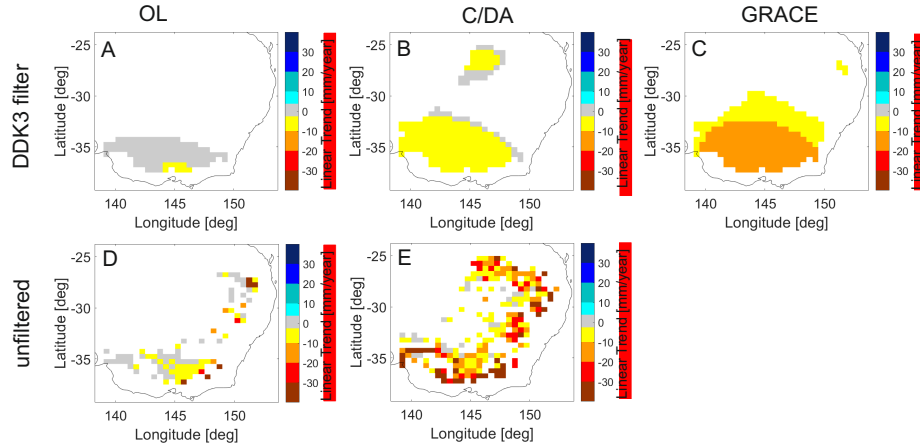


Figure 7: An overview of statistically significant linear trend in TWSC (in mm/year) within the MDB during 2003-2009. The results in (A), (B), and (C) are respectively derived after applying the DDK3 filter to the WGHM OL runs, improved WGHM after C/DA, and from ITSG-Grace2014. In (D) and (E), the linear trend from the original OL TWSC simulations of WGHM and after applying C/DA without any spatial filtering are shown, respectively.

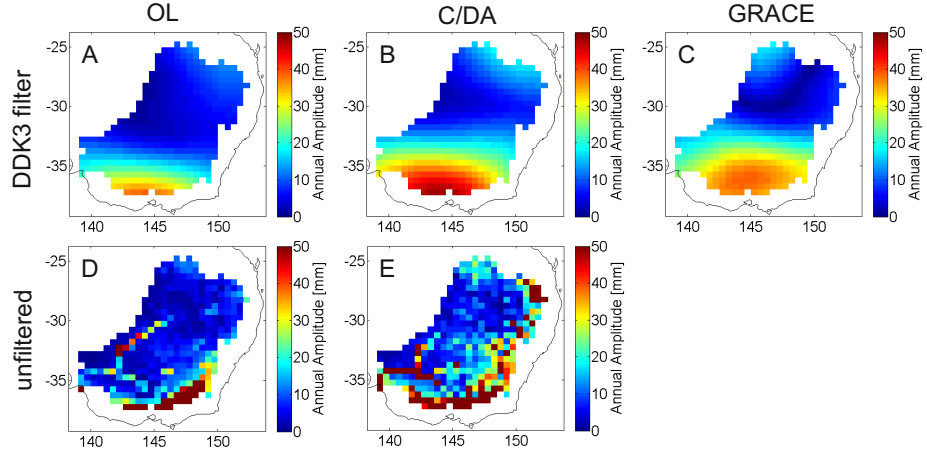


Figure 8: Annual amplitude of TWSC (in mm) from WGHM and GRACE. The DDK3-filtered results are shown in (A) using WGHM OL, (B) using improved WGHM after C/DA, and (C) using ITSG-Grace2014. In (D) and (E), the annual amplitudes from the original OL TWSC simulations of WGHM and after applying C/DA without any spatial filtering are shown, respectively.

negative linear trends are merged towards groundwater observations. The correlation coefficients of the OL and C/DA time series with respect to the groundwater observation time series are shown in Tab. 6.

The correlation coefficients are found to be even higher for the C/DA (v2) variant except for the south-western Murray region. The groundwater changes from the OL are found to be phase shifted compared to the wells observations, especially over the Murray sub-basins. As a result, small correlation coefficients are found between them. After C/DA, the phase shift is reduced over all regions except for the north-eastern Darling Basin (NE). The improvements occur mainly during 2006-2009, which are reflected in the higher correlation coefficients (Tab. 6). However, the inter-annual variability during 2003-2005 seems to be clearly underestimated in all regions. In 2010, the increase in groundwater is not yet captured by the C/DA variants that calibrate all 22 WGHM parameters. In contrast, the C/DA (v2) is able to reflect this increase in the groundwater compartment since the adjusted parameters are more efficient.

Groundwater observations are provided to us on $1^\circ \times 1^\circ$ grid cells. Thus, the OL and C/DA groundwater simulations are averaged on the same grid and the correlation coefficients before and after C/DA are shown in Fig. 10. Correlation

477 coefficients are found to be increased in some grid points, while for others no
 478 changes are observed. C/DA (v2) further improves the correlation coefficients
 479 over the Darling and Murray regions.

Table 6: Correlation coefficients between WGHM simulated groundwater changes (OL and after C/DA) and well measurements covering 2003-2009. MDB and its sub-basins are defined according to Fig. 1.

Basin	OL	ITSG-DDK3	C/DA (v2)
MDB	0.53	0.66 (+0.13)	0.72 (+0.19)
NW	-0.01	0.74 (+0.75)	0.82 (+0.83)
NE	0.32	0.16 (-0.17)	0.28 (-0.04)
SE	0.01	0.36 (+0.34)	0.41 (+0.39)
SW	-0.05	0.77 (+0.82)	0.69 (+0.75)

480 4.3.2. Spatial Distribution of the Groundwater Depletion

481 In Fig. 11 (A), (B) and (C), statistically significant linear trends in ground-
 482 water changes from the OL and C/DA variants of WGHM and the well mea-
 483 surements are shown. The OL simulation shows no trend in the majority of the
 484 grid cells. Assimilating ITSG-DDK3 TWSC observations into WGHM, restores
 485 negative trends to more than half of the grid cells. These trends correspond well
 486 to the linear trends derived from groundwater well measurements, which show
 487 strong linear trends (up to more than 40 mm/year) predominantly in the north
 488 and the south-east of the MDB. Also for the original WGHM groundwater time
 489 series on the $0.5^\circ \times 0.5^\circ$, OL shows no linear trend nearly all over the MDB (Fig.
 490 11 (D)). The more highly resolved grid values show that assimilating GRACE
 491 TWSC restores a negative trend predominantly in the north, east and south-
 492 east of the MDB (Fig. 11 (E)). Several grid cells especially in the south-east
 493 exhibit water decline of more than 40 mm/year. In case of C/DA (v2), the
 494 linear trends restored to the groundwater compartment are smaller for various
 495 grid cells compared to Fig. 11 (E) but considerably improved compared to the

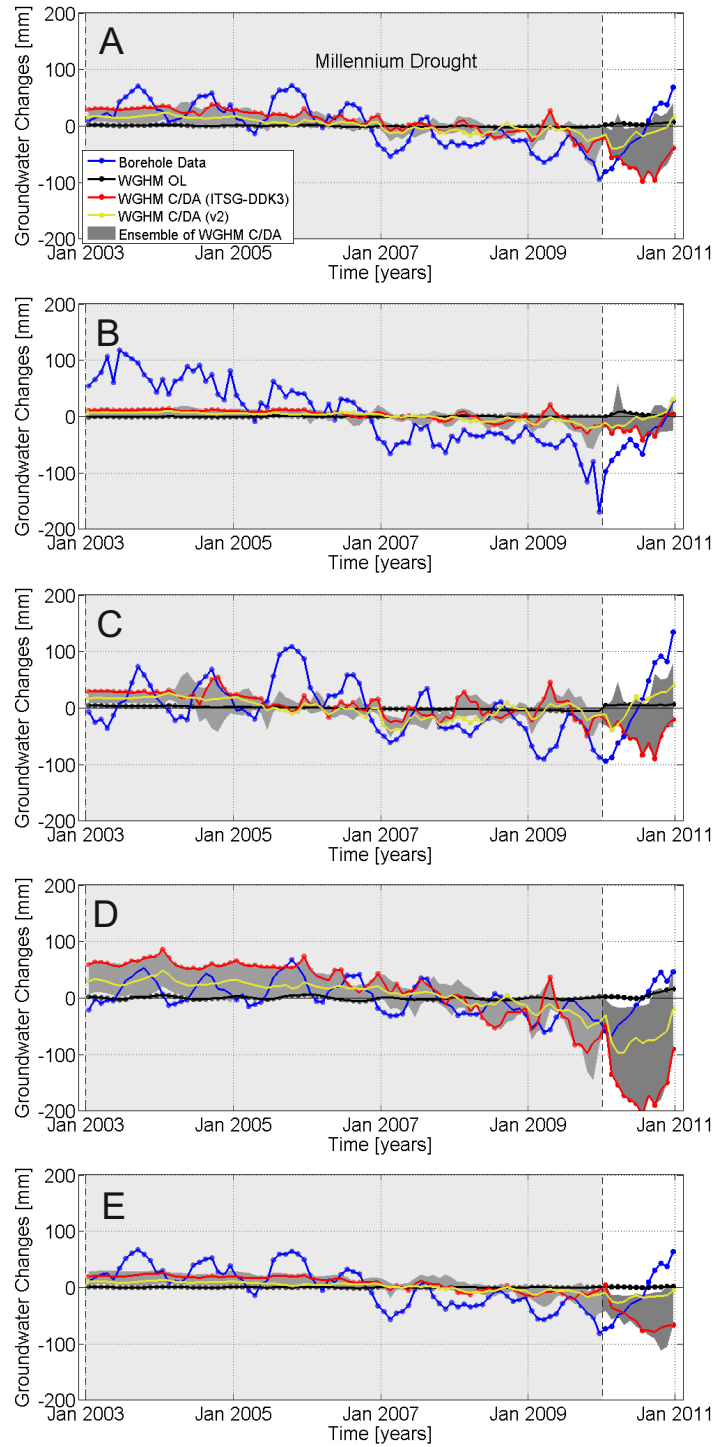


Figure 9: Monthly time series of groundwater changes (in mm) averaged (A) over the entire MDB, (B) over NW, (C) over NE, (D) over SE, and (E) over SW. The blue line indicates the groundwater observations; the black line indicates the WGHM OL simulation; the red line indicates the WGHM simulation after C/DA of GRACE (ITSG, DDK3), and the yellow line the WGHM simulation after C/DA (v2) of GRACE (ITSG, DDK3). The gray area represents the range of all C/DA results (see Tab. 2 for C/DA configurations).

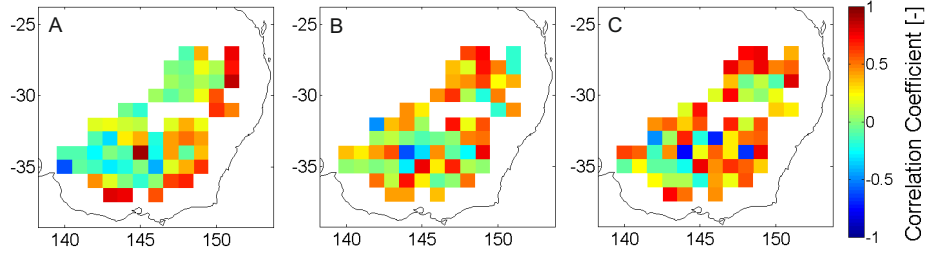


Figure 10: Correlation coefficients between wells data and: (A) the OL groundwater simulations, (B) the C/DA simulations (case ITSG-DDK3 while calibrating all 22 model parameters), and (C) the C/DA (v2) simulations (calibrating only 3 parameters).

OL variant.

The spatially averaged linear trends for the MDB and its four sub-basins are reported in Tab. 7. We have good confidence in the spatial averages of GRACE-derived TWSC over large areas such as the sub-basins of the MDB and their spatial distributions. These are accordingly integrated into the WGHM after C/DA. In contrast, the spatial averages over large areas from in-situ groundwater measurements are strongly influenced by interpolation errors, especially if well observations are obtained close to irrigation wells. More generally, groundwater observation wells tend to be positioned in reliable and productive aquifers. These may occupy only a small part of the landscape, and thus are not representative for the entire MDB (Tregoning et al., 2012, chapters 5 and 6). The ranking based on GRACE and the C/DA variants of WGHM also fits well to the spatial distribution of the difference in mean annual precipitation. Thus, it seems justified to trust the GRACE observations more than the groundwater well interpolation at large scales.

As for the estimation of linear trends in TWSC after C/DA, the choice of GRACE products and filtering clearly affects the linear trends in groundwater, which reaches up to 2 mm/year averaged over the entire MDB. The smallest impact of up to 1 mm/year occurred in the north-western Darling Basin (NW), which also exhibits the smallest linear trend among the sub-basins. In contrast, the linear trend in the south-eastern Murray Basin (NE) is affected by more

517 than 6 mm/year.

518 In order to demonstrate the impact of post-processing of groundwater mea-
519 surements on the validation of results, we modify the post-processing in two
520 ways: First, instead of using an average specific yield value of 0.1, values based
521 on a geology map are applied to convert groundwater levels to equivalent wa-
522 ter heights (Viney et al., 2015), i.e. values between 0.06 and 0.30; Second, we
523 identify those (gridded) groundwater time series that exhibit the highest RMSE
524 compared to the sub-basin averaged time series. It is assumed that these time
525 series might be representative for the $1^\circ \times 1^\circ$ grid cell but not for the sub-basin
526 average. Therefore, these grids are neglected and the sub-basin averages are
527 recomputed. From the different post-processing strategies an average water
528 storage decline of -11.6 mm/year is determined with a standard deviation of
529 ± 6.5 mm/year within the south-eastern Murray Basin (SE) and an average
530 decline of -33.3 mm/year with a standard deviation of ± 14.5 mm/year within
531 the north-western Darling Basin (NW; see last column in Tab. 7). These large
532 differences indicate the high dependency of the groundwater estimations on the
533 choice of specific yield and on the errors for computing (sub-)basin averages
534 from point measurements. The effect is found to be considerably higher than
535 the effect of the chosen GRACE product and the choice of the TWSC filtering
536 approach.

537 4.4. Model Parameter Calibration

538 An extensive section is provided in the Supplementary Data to discuss the
539 calibration of all the 22 WGHM parameters within the C/DA against calibrating
540 only the 3 parameters of the root depth multiplier, the net radiation multiplier,
541 and the groundwater outflow coefficient, which the implementation is called
542 C/DA (v2) from now on. We also modify a priori PDFs of the wetland and lake
543 depth and the groundwater outflow coefficient based on the investigation of the
544 update increments (see Tab. 1). The calibrated parameter values are shown
545 in Sect. 8 of the Supplementary Data. In general, our results indicate that by
546 calibrating all 22 parameters in some instances one can find few of them that

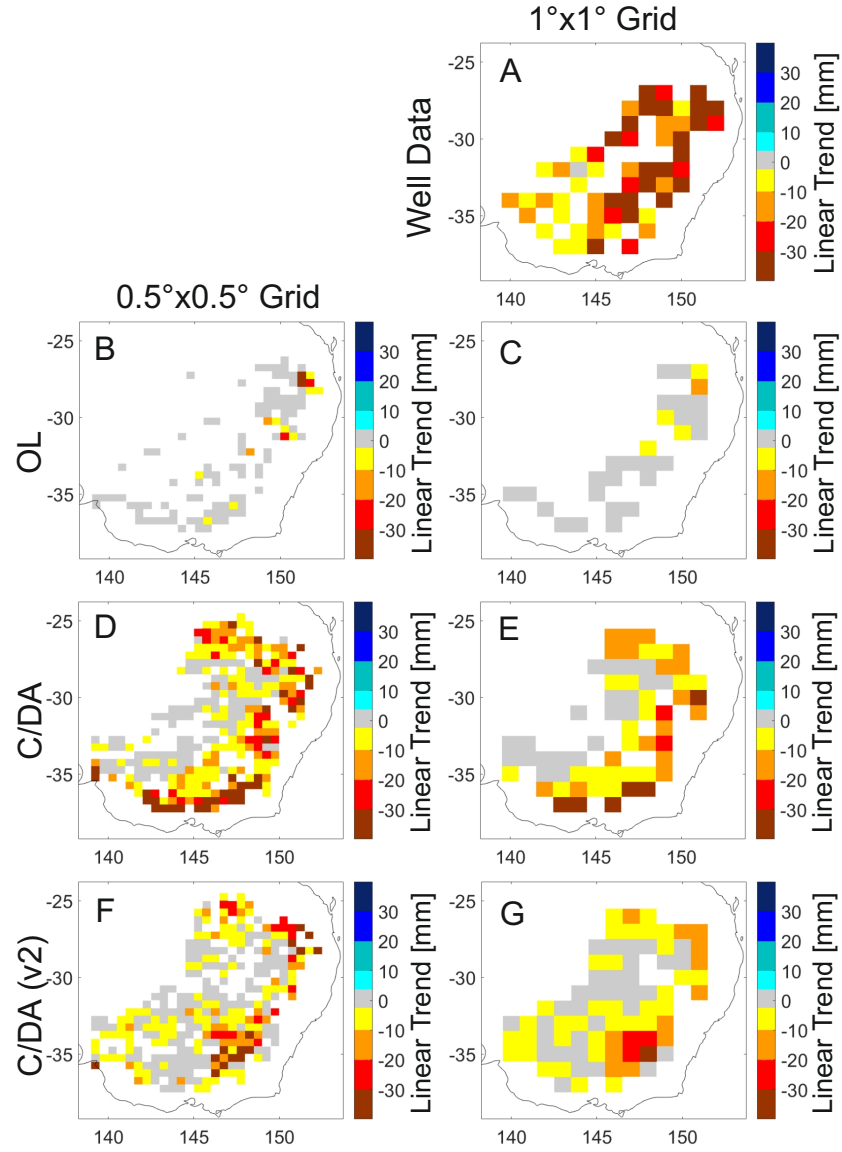


Figure 11: Significant linear trend in groundwater changes (in mm/year) within the MDB during 2003-2009. The results in (A), (C), (E) and (G) are respectively derived from the groundwater measurements, the WGHM OL, WGHM after C/DA while calibrating all 22 parameters, and from WGHM after C/DA (v2) while calibrating only 3 parameters. Results are spatially averaged over $1^\circ \times 1^\circ$ grid cells. In (B), (D), and (F), the linear trend from the original OL groundwater simulations of WGHM and after applying C/DA and C/DA (v2) are shown, respectively.

Table 7: Linear trends (in mm/year) in groundwater changes and their uncertainties during 2003-2009 computed for the entire MDB and the four sub-basins. The linear trends estimated from groundwater measurements (specific yield = 0.1) are provided in the second column. The results of WGHM OL and after C/DA of ITSG-DDK3 are shown in the third and fourth columns, respectively. The averages of linear trends and standard deviations from different GRACE products, and after applying different filtering techniques are reported in the fifth and sixth columns, respectively. The results of C/DA (v2) are provided in the seventh column. In the last column, the averages of linear trends and standard deviations from different post-processing strategies (specific yield modification, removing outliers) for the groundwater measurements are shown.

Basin	Data	OL	ITSG-DDK3	GRACE Product	GRACE Filtering	C/DA (v2)	Groundwater Variant
MDB	-16.1	-0.6 \pm 0.01	-8.3 \pm 0.2	-7.7 \pm 2.4	-5.9 \pm 2.2	-5.4 \pm 0.1	-20.5 \pm 4.0
NW	-28.7	0.1 \pm 0.00	-3.6 \pm 0.2	-4.5 \pm 1.0	-2.9 \pm 0.8	-3.1 \pm 0.1	-33.3 \pm 14.5
NE	-12.6	-1.4 \pm 0.02	-6.4 \pm 0.5	-5.2 \pm 2.5	-5.0 \pm 1.4	-5.6 \pm 0.1	-22.5 \pm 15.6
SE	-8.4	-0.4 \pm 0.02	-19.2 \pm 0.6	-16.3 \pm 6.3	-12.1 \pm 6.3	-9.6 \pm 0.1	-11.6 \pm 6.5
SW	-14.9	-0.1 \pm 0.01	-5.8 \pm 0.3	-7.2 \pm 1.6	-4.8 \pm 1.0	-3.4 \pm 0.1	-14.7 \pm 9.5

are not converged to a value within a priori range, while in C/DA (v2), all three parameters converge and their uncertainties are considerably reduced. This does not however necessarily imply that one version is better suited to achieve more accurate water storage simulations. Therefore, in the following, we mainly focus on interpreting the C/DA results derived from both versions.

The C/DA update increments, i.e. the difference between model prediction and model update, of the total and individual water storage compartments are presented in Fig. 12. Since mass is not conserved in the EnKF updates, these increments indicate how the water mass balance is violated by data assimilation (see also Sect. 5 of the Supplementary Data). The updates of soil water are higher in the east and south-east of the MDB, and decrease in western direction (Fig. 12 (B)). For groundwater, the same spatial pattern is visible but the amount of water mass associated with the groundwater compartment is considerable larger (Fig. 12 (C)). In Sect. 4.3, it is already shown that the updates for the groundwater compartment lead to improved agreements with in-situ observations. In addition, the updates for the soil water compartments

improve the seasonal representation of simulated TWSC after C/DA compared to the OL results (see Fig. S1 in the Supplementary Data). We find only small update increments for lakes, which seems to be reasonable, since only a few small surface water bodies are located in the MDB (Fig. 12 (D)).

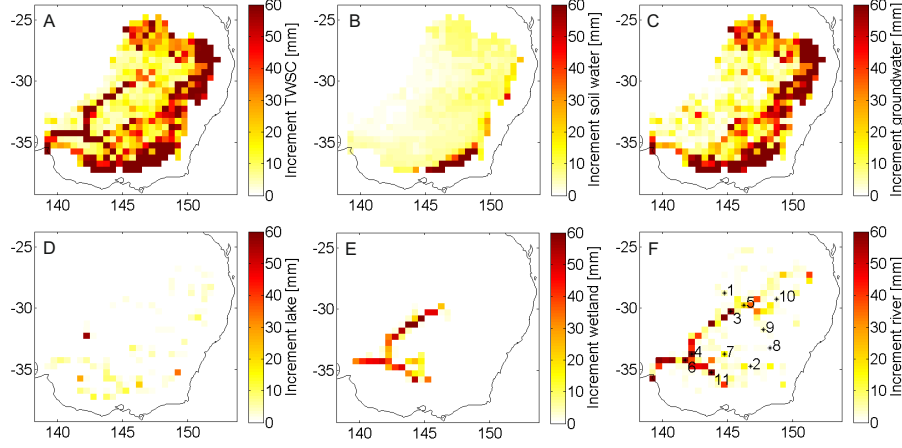


Figure 12: Root mean square (RMS) of monthly update increments after applying the C/DA to integrate WGHM with TWSC from ITSG-DDK3 (calibrating all 22 parameters) for (A) TWSC, (B) soil water, (C) groundwater, (D) lakes, (E) wetlands, and (F) rivers. In (F), the locations of the river discharge stations that have been used to calibrate the WaterGAP 2.2 model version are shown by the black dots.

4.5. River Discharge and River Level

To answer the Objective (5) of this paper, in sections 4.2 and 4.3, we showed how the C/DA improves total and individual water storage simulations of WGHM. Further insights will be provided in section 5. In this section, the impact of C/DA on WGHM’s river discharge and river level (storage) simulations is provided. Since GRACE data have a direct influence on water storage simulations and indirectly change simulated fluxes (e.g., river discharge, see Schumacher et al., 2015), one only needs to show the latter has not been worsen by the C/DA.

We use river discharge observations provided by the Bureau of Meteorology (BoM, <http://www.bom.gov.au/waterdata/>) to validate the updated river

578 compartment. In Fig. 13, the time series of river discharge are shown for three
579 selected stations while calibrating 22 parameters in (A), (C) and (E), as well as
580 for the C/DA (v2) in (B), (D) and (F). At the Paroo River at Caiwarro (BoM
581 station number 424201A; number 1 in Fig. 12 (F)), the WGHM OL simulated
582 river discharge fits quite well to the observations but the high flows in 2004,
583 2008 and 2010 are underestimated (Fig. 13 (A)). After performing the C/DA
584 run with 22 parameters, the discharge values represent the high flows better
585 than OL.

586 For other stations, the river compartment is found to be overestimated e.g.,
587 during 2003-2004, 2008-2009, and during the wet year 2010. In Fig. 13 (B)
588 and (C), we show the time series at Darling River at Burtundy (BoM station
589 number 425007; number 4 in Fig. 12 (F)) and Lachlan River at Booligal (BoM
590 station number 412005, number 7 in Fig. 12 (F)) as examples. After reducing
591 the number of calibration parameters, i.e. within the C/DA (v2) run, the river
592 discharge simulation is found to be improved. At Caiwarro (Fig. 13 (B)), the
593 high flows in 2004 and 2008 are better represented compared to the OL and
594 the previous C/DA run. However, in spring 2008 still two peaks are simulated
595 although only one of them is observed. At the other river discharge station, the
596 simulations are also improved. The high flows in 2010 are found to be much
597 closer to the observations for the C/DA (v2) run, especially at Burtundy (Fig.
598 13 (F)) but during the drought period they are still found to be overestimated.

599 We also compare simulated river storage with a number of stations provided
600 by the Murray-Darling Basin Authority ([https://riverdata.mdba.gov.au/
601 system-view](https://riverdata.mdba.gov.au/system-view)). For example, in Fig. 14, river storage outputs from WGHM
602 are compared with the time series of level changes derived from Murray's up-
603 stream, which is close to station 4 in Fig. 12(F). The comparison is limited to
604 2007.5-2011 during which the gauge data is available. Our results indicate that
605 the open-loop river storage is not well compared with observations (RMSE of
606 1.42), for example, high peaks are detected in 2008 and 2010, which are not
607 found in the measured levels. After applying the C/DA (both versions, how-
608 ever, the mentioned peaks are vanished and the general evolution of estimated

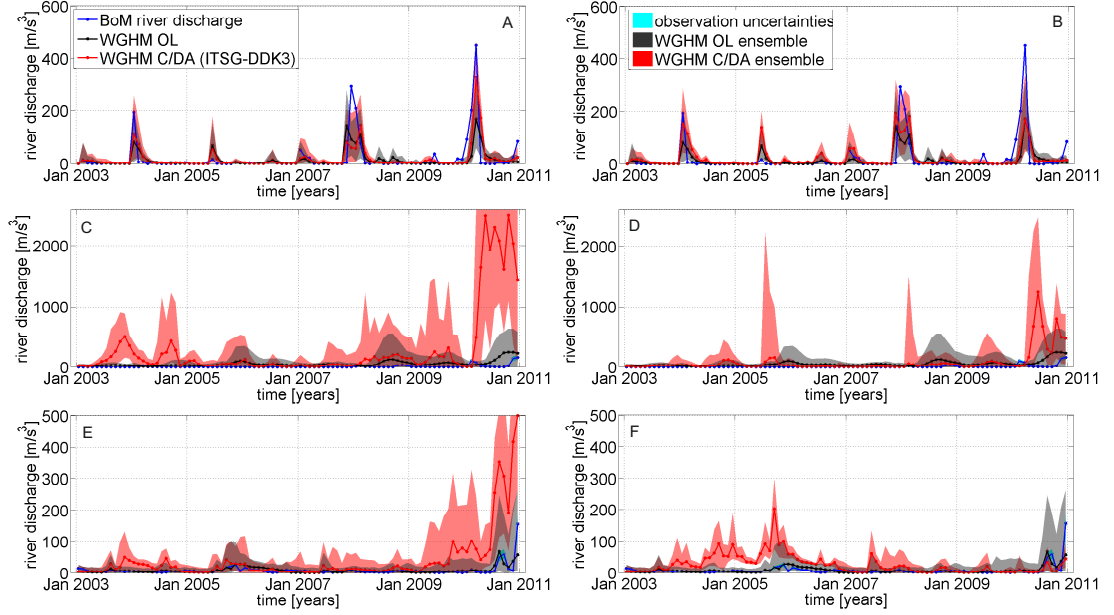


Figure 13: Time series of river discharge (in m^3/s) at three selected river discharge stations: (A, B) Paroo River at Caiwarro (BoM station number 424201A; number 1 in Fig. 12 (F)), (C, D) Darling River at Burtundy (BoM station number 425007; number 4 in Fig. 12 F); and (E, F) Lachlan River at Booligal (BoM station number 412005, number 7 in Fig. 12 (F)). The left column presents C/DA results from the ITSG-DDK3 case for which all 22 parameters have been calibrated, and the right column presents the C/DA (v2) while calibrating only 3 parameters.

609 river storage fairly well follows that of the gauge data, i.e., RMSE reduces to
 610 0.6. Correlation coefficients between the OL river level simulations and gauge
 611 observations indicate a weak correspondence of 0.15 (p-value showed that this
 612 correlation is not significant). This is increased to the statistically significant
 613 value of 0.52 (significant according to p-values) after implementing the C/DA.
 614 Impact of the 2010's La Niña is fairly well reflected in the C/DA derived river
 615 storage (compare the red and yellow curves in Fig. 14 with the observation
 616 curve in blue). Comparable results are found for the downstream station, which
 617 is not shown here.

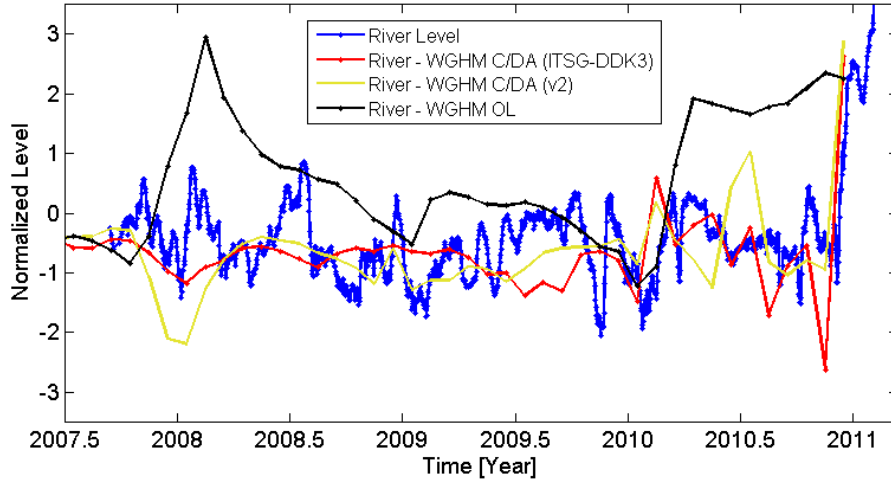


Figure 14: Time series of river level at the station 4 in Fig. 12 (F). The time series are temporally normalized, thus, they are unit-less.

618 5. Discussion

619 5.1. Choice of GRACE Product and Post-Processing

620 Several GRACE products (ITSG-Grace2016, GFZ, and JPL) with different
 621 spatial filters (the isotropic Gaussian and the anisotropic DDK filter) are as-
 622 sessed within the proposed C/DA in the MDB. Our analysis of the updated
 623 TWSC and groundwater changes is not able to suggest a single product or spa-
 624 tial filtering strategy that exhibits always superior metrics (here in terms of

RMSE and correlation coefficients). The magnitude of the differences among the EnKF variants is similar to the magnitude of the differences between the considered GRACE variants itself. The uncertainty information obtained for the ITSG-DDK3 results represents these differences among the EnKF variants fairly well. Thus, a careful incorporation of the GRACE TWSC uncertainty information provides reliable information of the spread of the EnKF updates that might have been obtained when selecting another data product.

5.2. *Effect of Equifinality of Calibration Parameters on C/DA Results*

We test calibrating only three parameters within the C/DA in order to mitigate the equifinality problem. We find that the three selected parameters converge to a constant value during the drought period and their uncertainty is clearly reduced. Although, improvements are already found for groundwater simulations during the drought period when calibrating 22 model parameters, it is not possible to constrain these many parameters using GRACE to improve the simulation of individual water storages when climate conditions rapidly and strongly change, i.e. the occurrence of strong rainfall events in 2010 after a long drought. This is, however, achieved by reducing the number of calibrated parameters. As a result, we find a strong positive impact on the EnKF updated of groundwater changes, especially in 2010.

In summary, parameter updating using GRACE observations is very challenging. Due to its current coarse spatial resolution and highly correlated errors, it might have limitations and might result in poorly constrained WGHM parameters that actually steer the simulation of individual water storage compartments or fluxes. An improved spatial resolution, which is expected from the GRACE follow on (GRACE-FO) mission (scheduled launch at the end of 2017), and a combination with other remote sensing observations might lead to better constrained parameter values.

5.3. *Application of the C/DA Framework within a (semi-)arid River Basin*

We find that all the EnKF variants improve the WGHM simulations and outperform the original simulations in terms of RMSE and correlation for the

655 (semi-)arid basin of the Murray and Darling rivers and its four sub-basins, and
656 even on the $0.5^\circ \times 0.5^\circ$ grid. The WGHM grid is much finer resolved than the
657 spatial resolution of GRACE data and therefore this result is not self-evident.
658 We would like to recall that we integrated GRACE data averaged over the
659 four major sub-basins of the MDB and not at each individual WGHM grid
660 point. Thus, the results give confidence that GRACE data can be horizontally
661 downscaled by the C/DA within (semi-)arid regions.

662 The water decline is primarily associated with the groundwater compart-
663 ment, which is confirmed through validation with independent well measure-
664 ments. However, in three out of the four MDB sub-basins, the restored trends
665 are much smaller than the observed ones. For a realistic assessment of the
666 C/DA performance, it is important to be aware that uncertainties exist also
667 for the ground-based validation data and these should not be treated as truth.
668 Thus, a perfect agreement between groundwater simulations after C/DA and
669 groundwater measurements cannot be expected. Using groundwater simulations
670 improved by C/DA of GRACE data has therefore the advantage that no specific
671 yield estimate and no spatial interpolation are required. The results indicate
672 that the groundwater simulations in the Darling Basin (NE) are less improved
673 compared to other regions in terms of correlation coefficients. The hydrological
674 reason for this is a different behavior in terms of annual cycles between GRACE
675 TWSC and groundwater well observations in this region. In fact, seasonality
676 of GRACE TWSC is less pronounced in the Darling Basin (NE), but it is vis-
677 ible in the in-situ well measurements. Thus, C/DA is not able to correct the
678 seasonality of WGHM's groundwater simulations in this sub-basin.

679 No significant trends are found in the surface water and soil water storage
680 compartments after 2003, which is in agreement with the analysis performed in
681 [Leblanc et al. \(2009\)](#). If the water decline was solely climate related, we would
682 expect more or less similar rates of decline in the surface, soil and groundwater
683 compartments. Our investigations however suggest that anthropogenic influence
684 on the hydrological cycle, in form of groundwater abstraction, is the reason for
685 the significant water decline within a wide area of the MDB (see, e.g., Fig. S8

686 (C), in which the net abstraction multiplier for groundwater is mostly larger
687 than 1), which is supported by local reports (e.g., from the Australian Bureau
688 of Meteorology).

689 The impact of C/DA on TWSC in the northern and southern regions of the
690 MDB is found to be different. Stronger seasonal amplitudes in the south result
691 in higher correlation coefficients but also higher RMSE values. The response
692 of the hydrological resources within the four sub-basins to the meteorological
693 drought also differs for the northern and southern sub-basins. The spatial dis-
694 tribution of the BoM precipitation data shows that more rainfall occurred in the
695 northern MDB, especially in the Darling Basin (NW), compared to the other
696 sub-basins. Thus, the impact of the Millennium Drought is found to be pre-
697 dominant in the southern MDB, which is in agreement with the pronounced
698 hydrological drought in the south observed by GRACE. The negative linear
699 trends of TWSC, as well as groundwater are less strong in the north compared
700 to the south. The reason might not only be related to the climatological condi-
701 tions but also to the human influence on the water resources in the MDB. Due
702 to surface water subtractions, e.g., from the Darling River in the north, less
703 water enters the Murray sub-basins in the south. In order to ensure irrigation
704 and therefore continue agricultural activities, groundwater is even more heavily
705 pumped resulting in the observed decline of TWSC and groundwater resources.
706 This statement is supported by the engagement of the Murray Darling Basin
707 Authority (see <https://www.mdba.gov.au/>) that established a Basin Plan to
708 manage the entire basin as one system beyond political borders in order to
709 balance the water use and to ensure a sustainable use of the water resources.
710 The hydrological drought is therefore a consequence of the mixture of dry mete-
711 orological conditions and human impact on the water cycle, which is especially
712 pronounced in the southern MDB.

713 According to the results we show above, we are confident to state that the
714 C/DA approach can be applied to use GRACE and improve a model (here
715 WGHM) in a (semi-)arid region without tuning its setting. However, few prob-
716 lems remain for the simulation of river discharge. It is important to keep in

mind that assimilating GRACE data into a model does not directly affect the river discharge simulation but rather through the calibration of several model parameters. Therefore, a perfect agreement with river discharge observations for the entire basin cannot be expected at least by the current resolution of GRACE products. However, after applying the C/DA we find a good agreement between river storage simulation of WGHM and gauge observations at the Murray's upstream and downstream. Therefore, our conclusion is that the C/DA successfully improves storage simulation of WGHM. To achieve better discharge simulations, one likely needs to assimilate observations in the form of water fluxes (e.g., river flow and/or multiple altimetry observations), which will be addressed in future.

5.4. *Groundwater and Soil Storage Response to Climate Variability and Water Abstraction*

In this section, we explore the spatial and temporal variability of soil water storage and groundwater changes within the entire Murray Darling Basin by applying a principal component analysis (PCA, Forootan, 2014, chapter 3) on the outputs of WGHM before and after implementing C/DA. This analysis helps us to understand how these storages evolve after a dry season and how they response to climate variability.

In Figs. 15 and 16, PCA results of soil water and groundwater storage changes are shown, respectively. In both figures, the spatial patterns are empirical orthogonal function (EOF) in mm that can be interpreted as anomaly maps and their corresponding temporal evolutions are unit-less (normalized) evolutions shown on right and labeled as principal component (PC). By multiplying EOF and PC, one can reconstruct spatio-temporal variability of soil and groundwater storage changes in the region, while representing their maximum variance. Our computations indicate that the first mode of soil (EOF1 and PC1 of soil in Fig. 15) is equivalent with 62% of the total variance and the one of groundwater (EOF1 and PC1 in Fig. 16) represents 78% of the total variance. For brevity, in both Figs. 15 and 16, we only show the EOF that cor-

responds to the open loop output but PCs are estimated separately by applying
 PCA on the soil water and groundwater storage outputs of open loop, C/DA
 with all parameters, and C/DA with 3 parameters. The presentation of PCs is
 limited to the period of 2007.5-2011, within which the PCs are better distin-
 guishable. In both figures, we also show a measure of ENSO events, reflected
 in the southern oscillation index (SOI), which is downloaded from the website
 of BoM (<http://www.bom.gov.au/climate/current/soi2.shtml>). Sustained
 positive values of the SOI used here represent La Niña episodes and its negative
 values represent El Niño, which respectively correspond to higher and lower
 than normal precipitation in Australia.

PCA results of soil storage from the open loop output indicate stronger
 anomalies on the east and north parts of the basin (see EOF1 in Fig. 15), as
 well as a temporal delay of ~ 6 months between peaks of ENSO and soil moisture
 in 2008 and 2009. The strong La Niña in 2010 is found to change the open loop's
 soil storage outputs quite immediately. We find no obvious trend in the open
 loop results, which apparently indicate that the history of water storage does
 not play a major role in simulating the maximum peaks derived from WGHM
 (see the black curve in Fig. 15). PCs derived from the C/DA outputs reflect the
 ENSO activity on the basin's soil water storage more realistically. Particularly,
 we find the dry period of 2008.8-2010.2 causes a decline in soil storage (covering
 2009.2-2010.6), which is recovered by the La Niña in the middle of 2010 (see the
 red and yellow curves in Fig. 15).

Application of C/DA is found very beneficial for improving the representa-
 tion of groundwater in the basin. The PCA results derived from groundwater
 output of the open loop run (see the black curve in Fig. 16) indicate a moder-
 ate decline until 2010, which is followed by a sudden groundwater recharge that
 is likely caused by the extensive rainfall in 2010-2011. Groundwater anoma-
 lies are found stronger along the river (see EOF in Fig. 16). The computed
 groundwater PCs, derived after implementing the C/DA (both versions), evolve
 more naturally than that of the open loop. For example, it is clear that within
 the La Niña years of 2007.5-2009.5, the rate of groundwater storage decline is

778 quite moderate (see the red and yellow curves in Fig. 16), which likely reflects
 779 the impact of water use. An accelerated groundwater depletion is found dur-
 780 ing 2009-2010.2, which reflects both a strong El Niño and extensive irrigations.
 781 Then, the water decline has been gradually recovered by the 2010's La Niña.

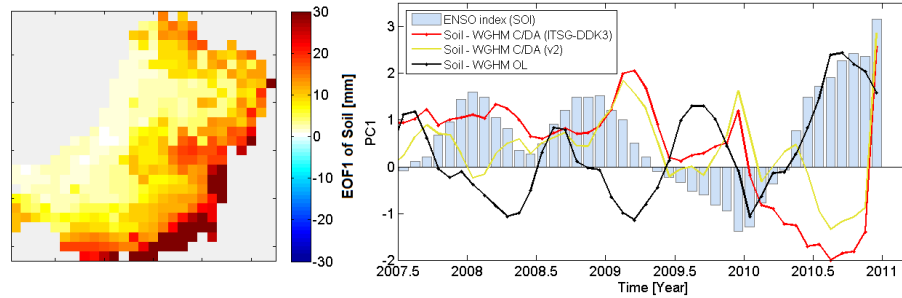


Figure 15: First dominant orthogonal mode, including EOF and its corresponding PC, derived from soil moisture outputs of WGHM. Here EOF1 is derived from the open loop run, but PC1 is derived by applying PCA on the open loop, and two versions of the C/DA outputs and compared to the ENSO index (SOI). This dominant mode represents 62% of variance in soil moisture variability in the region.

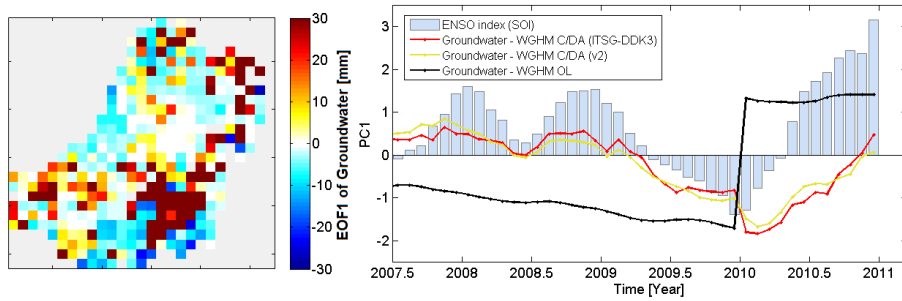


Figure 16: First dominant orthogonal mode, including EOF1 and its corresponding temporal pattern PC1, derived from groundwater outputs of WGHM is shown. Here EOF1 is derived from the open loop run, but PC1 is derived by applying PCA on the open loop, and two versions of the C/DA outputs and compared to the ENSO index (SOI). This dominant mode (EOF1 and PC1 together) represents 78% of variance in groundwater variability in the region.

782 6. Conclusions and Outlook

783 A novel calibration and data assimilation (C/DA) framework ([Schumacher](#)
784 [et al., 2016](#)) is applied here to integrate terrestrial water storage changes (TWSC)
785 observed by GRACE satellites into WGHM within the Murray-Darling Basin
786 (MDB) during 2003-2010. Several technical insights are revealed from this as-
787 sessment that are summarized in the following:

- 788 1. By applying the C/DA approach to the (semi-)arid region of the MDB,
789 it is possible to restore linear trends into WGHM, and also improve the
790 seasonality. As droughts in the MDB are well studied, they can act as
791 a reference for impact models like WGHM. The association of the water
792 decline with the correct water storage compartment, i.e. groundwater in
793 our study, is achieved and validated against ground-based well measure-
794 ments. Our results show that by implementing C/DA the response of soil
795 water and groundwater storage to climate variability within the MDB has
796 been improved. Our results indicate that although river discharge simu-
797 lation WGHM in the MDB cannot be improved by assimilating limited
798 resolution GRACE data, its river storage simulations can be considerably
799 (positively) influenced by the C/DA.
- 800 2. Difficulties exist when combining information from different sources, i.e.
801 model simulations, remote sensing and ground-based measurements, and
802 of different spatial resolution and accuracy. Uncertainties of ground-based
803 data have to be considered for independent validation of the C/DA per-
804 formance and a perfect agreement might not be expected.
- 805 3. Adapting the C/DA settings to basin-specific characteristics (in this study
806 by modifying a priori PDFs of parameters) and reducing the number of
807 calibration parameters to avoid equifinality has several positive impacts
808 on the C/DA results: (i) the uncertainties of calibration parameters are
809 clearly reduced and their values converge; (ii) the influence of climate
810 condition on the groundwater compartments is captured; and (iii) the

811 representation of river discharge is clearly improved, especially within the
812 wet year 2010.

- 813 4. The calibration of a smaller parameter sub-set clearly suggests that param-
814 eter values vary with changes of climatic conditions within the river basin.
815 Therefore, allowing the model parameters to change over time results in a
816 better representation of water storage variability and water fluxes within
817 MDB.
- 818 5. Parameter updating using GRACE observations is very challenging, even
819 if the number of calibration parameters is reduced. Combined C/DA using
820 GRACE data is a highly under-determined system that might be limited
821 in constraining individual model parameters, while an optimal parameter
822 set with respect to TWSC simulations is always achieved.
- 823 6. Comparing WGHM outputs with in-situ observations indicates that C/DA
824 of GRACE data does not improve river discharge simulations in the MDB,
825 but river storage simulations are significantly improved. This is likely
826 caused by limitation in model equations that transfer storage information
827 to water fluxes (Müller Schmied et al., 2014). This limitation is not only
828 an issue for WGHM but also most of existing hydrological or land surface
829 models.
- 830 7. Comparing GRACE data from different providers and using different fil-
831 tering techniques, it seems that their impact on the final C/DA results is
832 smaller than GRACE data errors.

833 The assessment of our C/DA approach for assimilating GRACE TWSC into
834 a hydrological model has clearly shown the strengths and limitations of the
835 current implementation. For future work, the application of a multi-criteria
836 C/DA approach in which data on river discharge and possibly surface water
837 level variations are taken into account might further help to improve the C/DA
838 results.

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849 and level, as well as climate indices used in this study.

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1058 **List of Figure Captions**

1059	1	The Murray-Darling Basin (MDB) and its four sub-basins con-	
1060		sidered here to integrate GRACE TWSC with the WGHM model	
1061		simulations.	9
1062	2	Set-up of study for the Murray-Darling Basin (MDB). First, open	
1063		loop (OL) model runs are performed over 2003-2010 (left column).	
1064		Subsequently, GRACE TWSC averaged over the 4 major sub-	
1065		basins of the MDB are assimilated into WGHM testing different	
1066		configurations (center and right column) and simultaneously the	
1067		WGHM's parameters are calibrated (see Tab 1). To assess the	
1068		C/DA results, simulated TWSC and groundwater changes are	
1069		compared to GRACE TWSC and independent groundwater well	
1070		measurements.	13
1071	3	(A) Divergence of annual precipitation in mm (from the long-	
1072		term temporal mean of 477 mm) averaged over the entire Murray-	
1073		Darling Basin (MDB). (B) Difference in mean annual precipita-	
1074		tion during 2001-2009 and 1981-2013 on a $0.5^\circ \times 0.5^\circ$ grid.	16
1075	4	TWSC (in mm) derived from the WGHM open loop (OL) run	
1076		and from GRACE averaged over the entire Murray-Darling Basin	
1077		(MDB). The black line shows the WGHM OL, the blue line in-	
1078		dicates GRACE (using ITSG-Grace2014), which is smoothed by	
1079		the DKK3 filter, while the dark gray area represents the range of	
1080		all investigated GRACE datasets (see Tab. 2).	17

1081	5	Monthly TWSC in mm averaged (A) over the entire MDB, (B)	
1082		over NW, (C) over NE, (D) over SE, and (E) over SW. The blue	
1083		line indicates the TWSC from GRACE (ITSG, DDK3); the black	
1084		line indicates the WGHM OL simulation; the red line indicates	
1085		the WGHM simulation after C/DA of GRACE (ITSG, DDK3),	
1086		and the yellow line the WGHM simulation after C/DA (v2) of	
1087		GRACE (ITSG, DDK3). The dark gray area represents the range	
1088		of all C/DA results (see Tab. 2 for C/DA configurations).	20
1089	6	Gridded correlation coefficients between WGHM TWSC simula-	
1090		tion and ITSG-Grace2014 TWSC after applying DDK3 filtering	
1091		for both; (A) for the OL, (B) after applying the C/DA. Gridded	
1092		root mean square error (RMSE) in mm estimated (C) from the	
1093		differences between OL TWSC and those of GRACE, and (D)	
1094		from the C/DA TWSC and GRACE TWSC.	21
1095	7	An overview of statistically significant linear trend in TWSC (in	
1096		mm/year) within the MDB during 2003-2009. The results in (A),	
1097		(B), and (C) are respectively derived after applying the DDK3	
1098		filter to the WGHM OL runs, improved WGHM after C/DA, and	
1099		from ITSG-Grace2014. In (D) and (E), the linear trend from the	
1100		original OL TWSC simulations of WGHM and after applying	
1101		C/DA without any spatial filtering are shown, respectively.	23
1102	8	Annual amplitude of TWSC (in mm) from WGHM and GRACE.	
1103		The DDK3-filtered results are shown in (A) using WGHM OL,	
1104		(B) using improved WGHM after C/DA, and (C) using ITSG-	
1105		Grace2014. In (D) and (E), the annual amplitudes from the orig-	
1106		inal OL TWSC simulations of WGHM and after applying C/DA	
1107		without any spatial filtering are shown, respectively.	24

1108	9	Monthly time series of groundwater changes (in mm) averaged	
1109		(A) over the entire MDB, (B) over NW, (C) over NE, (D) over	
1110		SE, and (E) over SW. The blue line indicates the groundwater	
1111		observations; the black line indicates the WGHM OL simula-	
1112		tion; the red line indicates the WGHM simulation after C/DA of	
1113		GRACE (ITSG, DDK3), and the yellow line the WGHM simula-	
1114		tion after C/DA (v2) of GRACE (ITSG, DDK3). The gray area	
1115		represents the range of all C/DA results (see Tab. 2 for C/DA	
1116		configurations).	26
1117	10	Correlation coefficients between wells data and: (A) the OL ground-	
1118		water simulations, (B) the C/DA simulations (case ITSG-DDK3	
1119		while calibrating all 22 model parameters), and (C) the C/DA	
1120		(v2) simulations (calibrating only 3 parameters).	27
1121	11	Significant linear trend in groundwater changes (in mm/year)	
1122		within the MDB during 2003-2009. The results in (A), (C), (E)	
1123		and (G) are respectively derived from the groundwater measure-	
1124		ments, the WGHM OL, WGHM after C/DA while calibrating all	
1125		22 parameters, and from WGHM after C/DA (v2) while calibrat-	
1126		ing only 3 parameters. Results are spatially averaged over $1^\circ \times 1^\circ$	
1127		grid cells. In (B), (D), and (F), the linear trend from the orig-	
1128		inal OL groundwater simulations of WGHM and after applying	
1129		C/DA and C/DA (v2) are shown, respectively.	29
1130	12	Root mean square (RMS) of monthly update increments after	
1131		applying the C/DA to integrate WGHM with TWSC from ITSG-	
1132		DDK3 (calibrating all 22 parameters) for (A) TWSC, (B) soil	
1133		water, (C) groundwater, (D) lakes, (E) wetlands, and (F) rivers.	
1134		In (F), the locations of the river discharge stations that have been	
1135		used to calibrate the WaterGAP 2.2 model version are shown by	
1136		the black dots.	31

1137	13	Time series of river discharge (in m/s^3) at three selected river	
1138		discharge stations: (A, B) Paroo River at Caiwarro (BoM station	
1139		number 424201A; number 1 in Fig. 12 (F)), (C, D) Darling River	
1140		at Burtundy (BoM station number 425007; number 4 in Fig. 12	
1141		F); and (E, F) Lachlan River at Booligal (BoM station number	
1142		412005, number 7 in Fig. 12 (F)). The left column presents C/DA	
1143		results from the ITSG-DDK3 case for which all 22 parameters	
1144		have been calibrated, and the right column presents the C/DA	
1145		(v2) while calibrating only 3 parameters.	33
1146	14	Time series of river level at the station 4 in Fig. 12 (F). The time	
1147		series are temporally normalized, thus, they are unit-less.	34
1148	15	First dominant orthogonal mode, including EOF and its corre-	
1149		sponding PC, derived from soil moisture outputs of WGHM. Here	
1150		EOF1 is derived from the open loop run, but PC1 is derived by	
1151		applying PCA on the open loop, and two versions of the C/DA	
1152		outputs and compared to the ENSO index (SOI). This dominant	
1153		mode represents 62% of variance in soil moisture variability in	
1154		the region.	40
1155	16	First dominant orthogonal mode, including EOF1 and its corre-	
1156		sponding temporal pattern PC1, derived from groundwater out-	
1157		puts of WGHM is shown. Here EOF1 is derived from the open	
1158		loop run, but PC1 is derived by applying PCA on the open loop,	
1159		and two versions of the C/DA outputs and compared to the	
1160		ENSO index (SOI). This dominant mode (EOF1 and PC1 to-	
1161		gether) represents 78% of variance in groundwater variability in	
1162		the region.	40